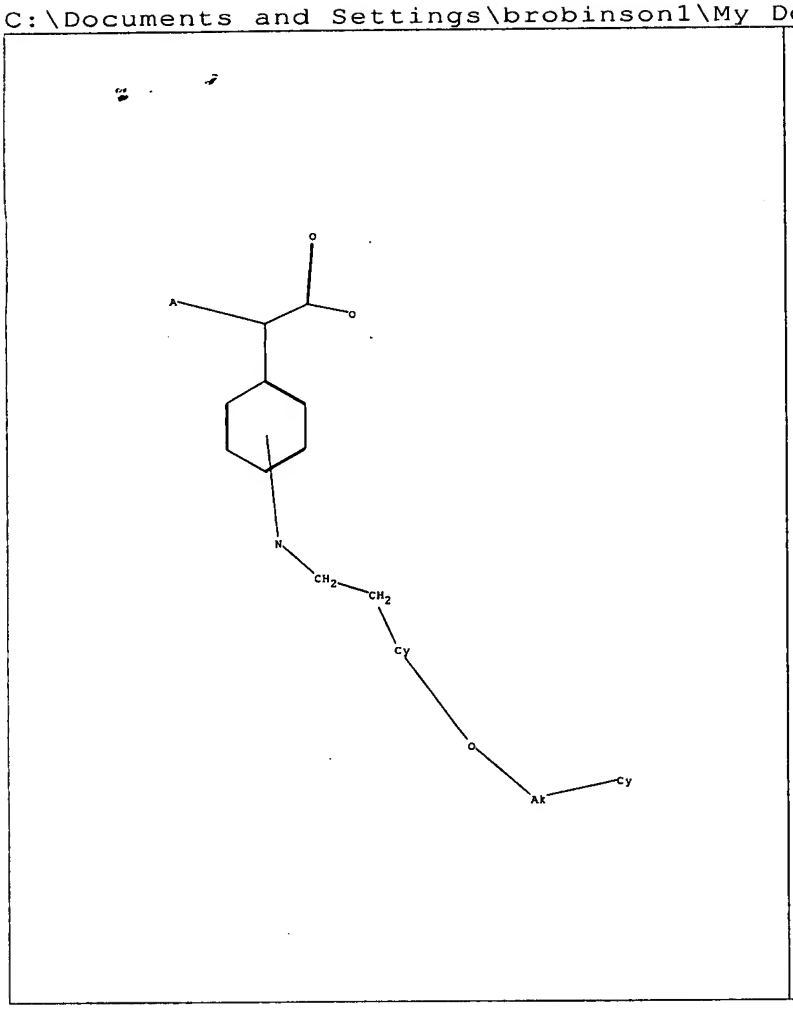
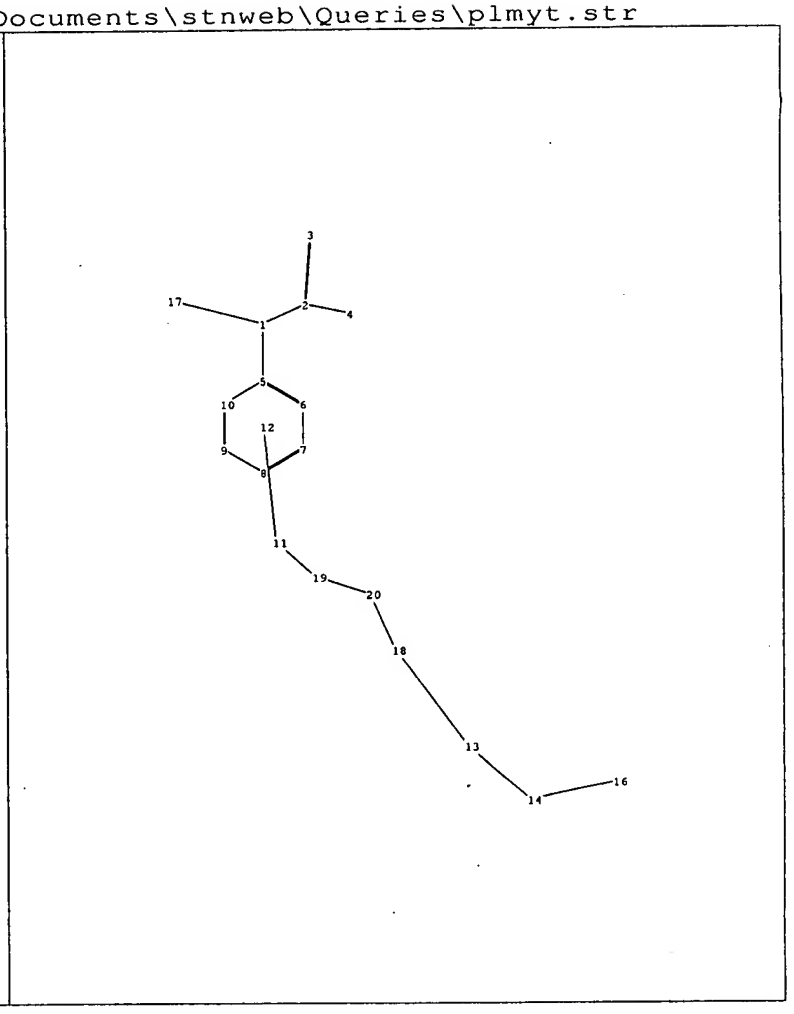
EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	907	(544/105).CCLS.	US-PGPUB; USPAT	OR	OFF	2007/04/06 19:13
L2	503	1 and carboxylic and acid	US-PGPUB; USPAT	OR	OFF	2007/04/06 19:13

C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\plmyt.str

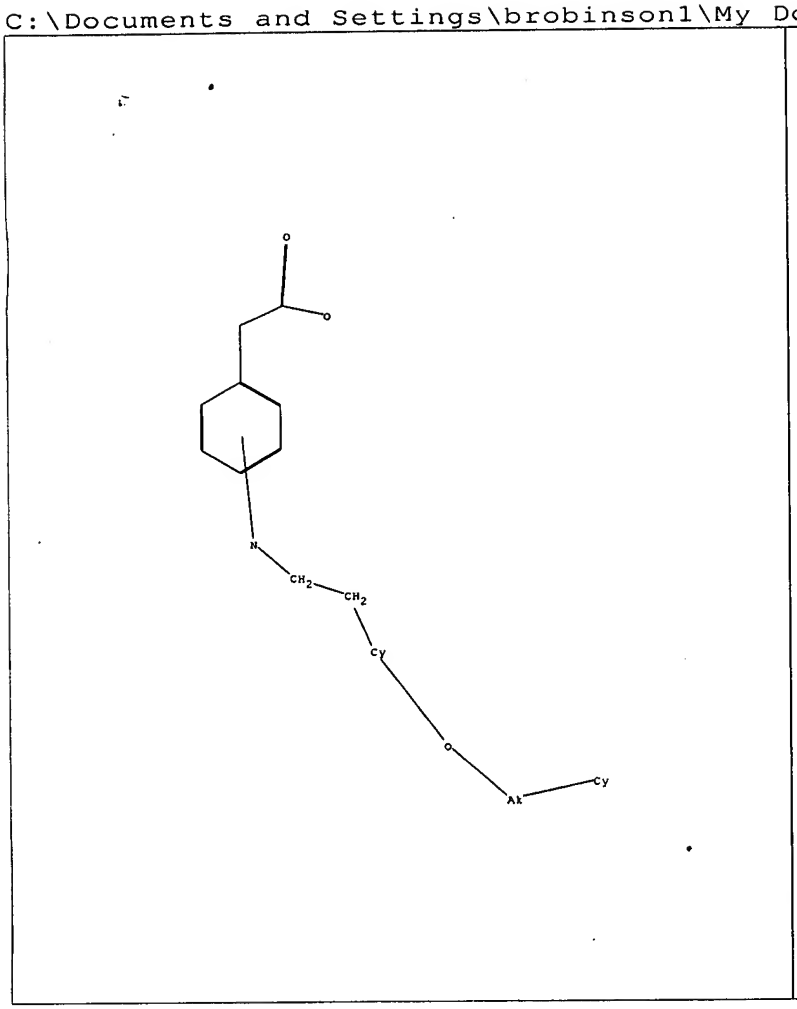


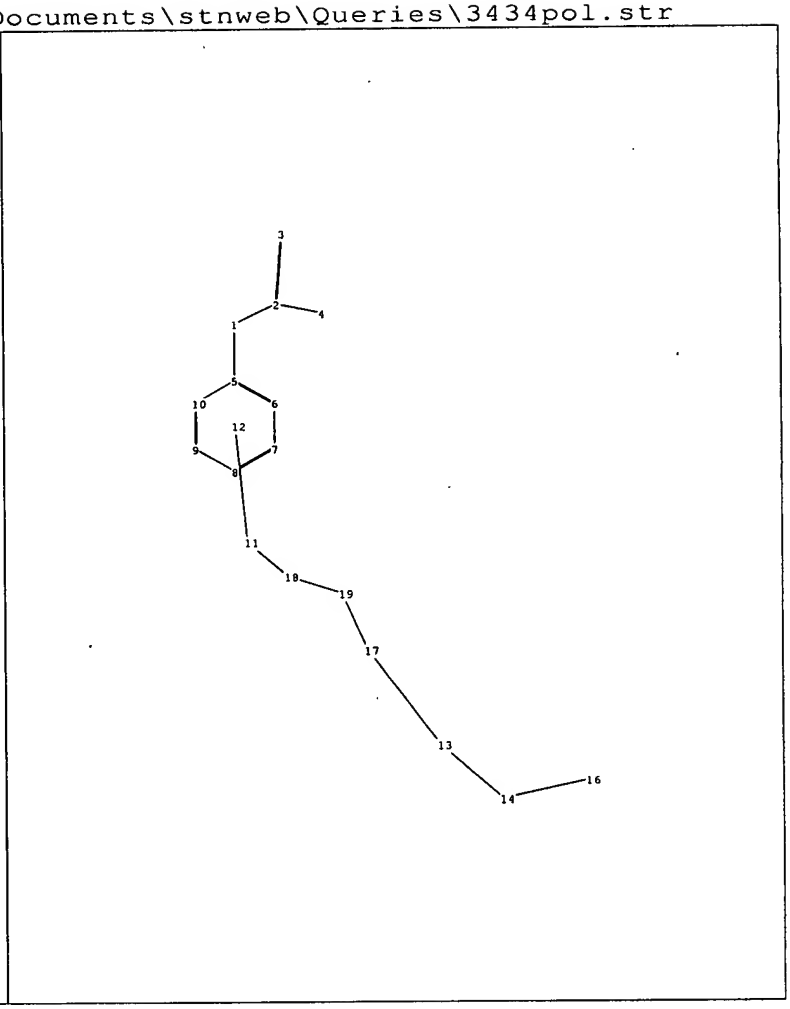


chain nodes :
1 2 3 4 11 13 14 16 17 18 19 20
ring nodes :
5 6 7 8 9 10
chain bonds :
1-2 1-5 1-17 2-3 2-4 11-19 13-14 13-18 14-16 18-20 19-20
ring bonds :
5-6 5-10 6-7 7-8 8-9 9-10
exact/norm bonds :
1-17 2-3 2-4 13-14 13-18 14-16 18-20
exact bonds :
1-2 1-5 11-19 19-20
normalized bonds :
5-6 5-10 6-7 7-8 8-9 9-10
isolated ring systems :
containing 1 : 5 :

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS 12:Atom 13:CLASS 14:CLASS 16:CLASS 17:CLASS 18:Atom
19:CLASS 20:CLASS

C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\3434pol.str





chain nodes :
2 3 4 11 13 14 16 17 18 19
ring nodes :
5 6 7 8 9 10
ring/chain nodes :
1
chain bonds :
1-2 1-5 2-3 2-4 11-18 13-14 13-17 14-16 17-19 18-19
ring bonds :
5-6 5-10 6-7 7-8 8-9 9-10
exact/norm bonds :
2-3 2-4 13-14 13-17 14-16 17-19
exact bonds :
1-2 1-5 11-18 18-19
normalized bonds :
5-6 5-10 6-7 7-8 8-9 9-10
isolated ring systems :
containing 1 : 5 :

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS 12:Atom 13:CLASS 14:CLASS 16:CLASS 17:Atom 18:CLASS
19:CLASS

10572578

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1612bxr

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'CAOLD' AT 17:04:25 ON 06 APR 2007
FILE 'CAOLD' ENTERED AT 17:04:25 ON 06 APR 2007
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.90	193.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.90	193.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

FILE 'REGISTRY' ENTERED AT 17:04:35 ON 06 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2007 HIGHEST RN 929247-80-3
DICTIONARY FILE UPDATES: 5 APR 2007 HIGHEST RN 929247-80-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\plmyt.str

Updated Search

10572578

L6 STRUCTURE UPLOADED

=> s l6
SAMPLE SEARCH INITIATED 17:06:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 14859 TO ITERATE

13.5% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 289879 TO 304481
PROJECTED ANSWERS: 0 TO 0

L7 0 SEA SSS SAM L6

=> s l6 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 17:06:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 298412 TO ITERATE

100.0% PROCESSED 298412 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.04

L8 0 SEA SSS FUL L6

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\3434pol.str

L9 STRUCTURE UPLOADED

=> s l9
SAMPLE SEARCH INITIATED 17:07:28 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 14859 TO ITERATE

13.5% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 289879 TO 304481
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

=> s l9 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 17:07:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 298412 TO ITERATE

100.0% PROCESSED 298412 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.04

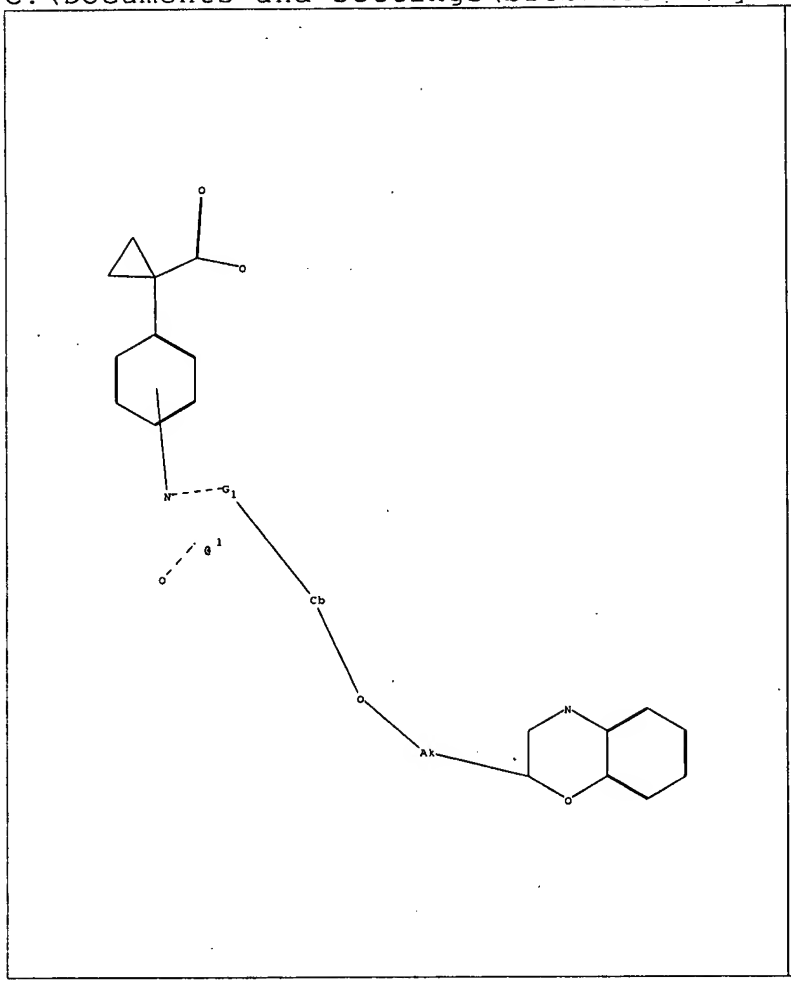
Updated Search

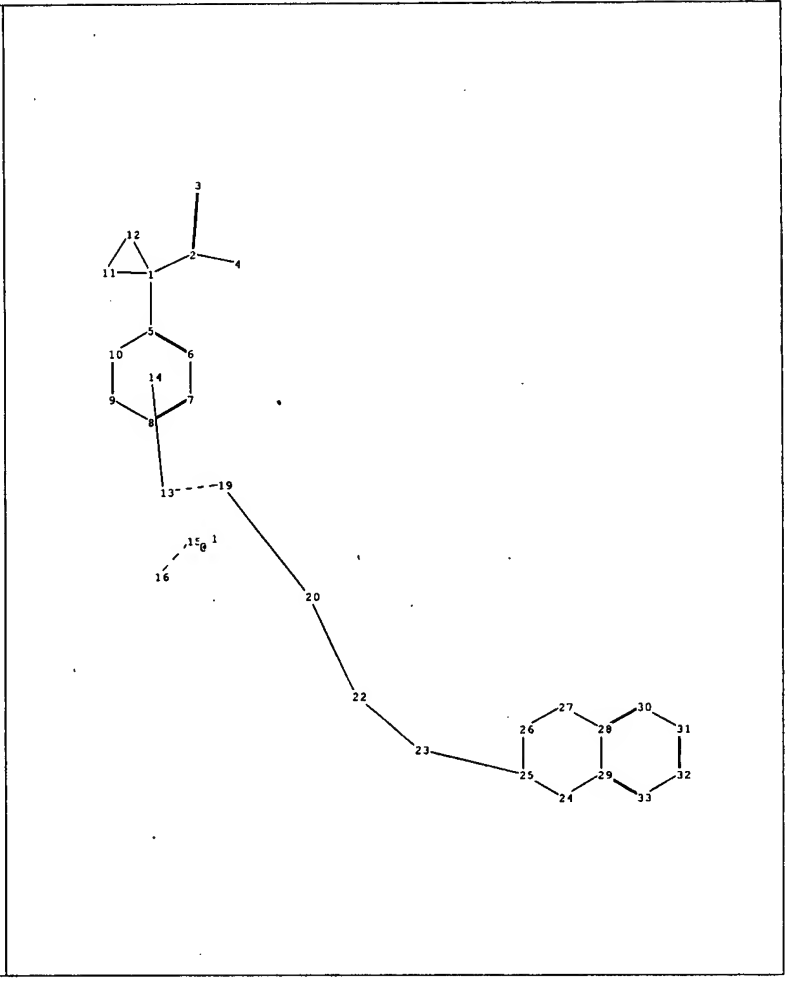
10572578

L11 0 SEA SSS FUL L9

Updated Search

C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\232329il.str



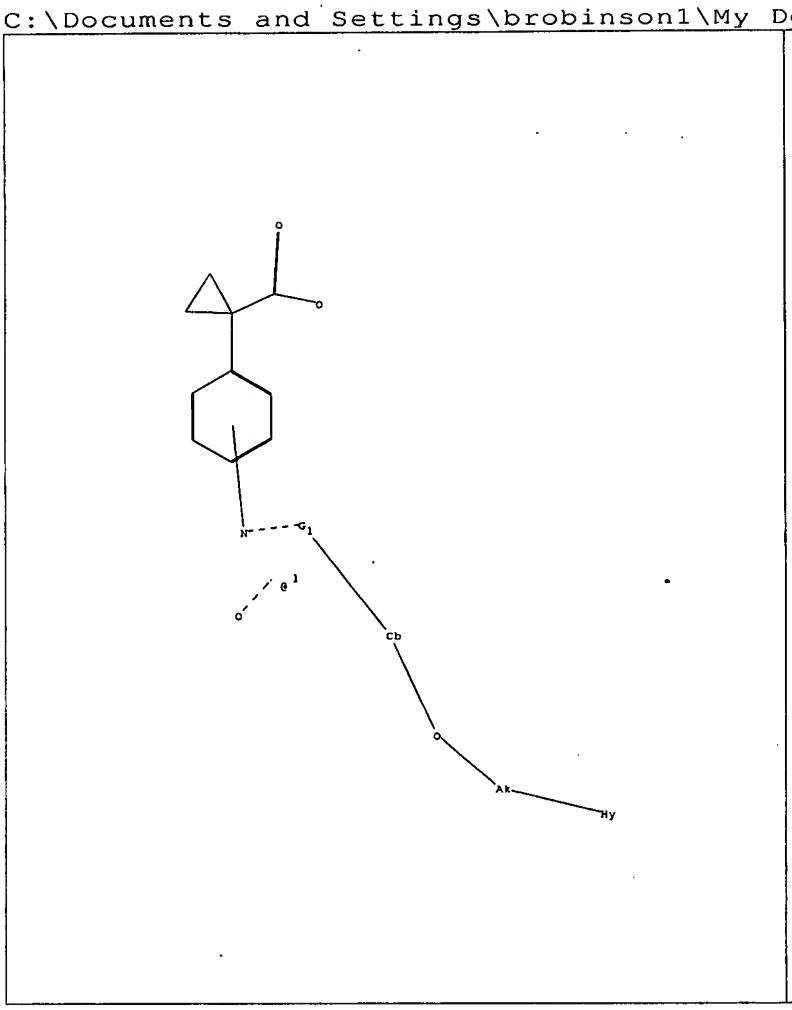


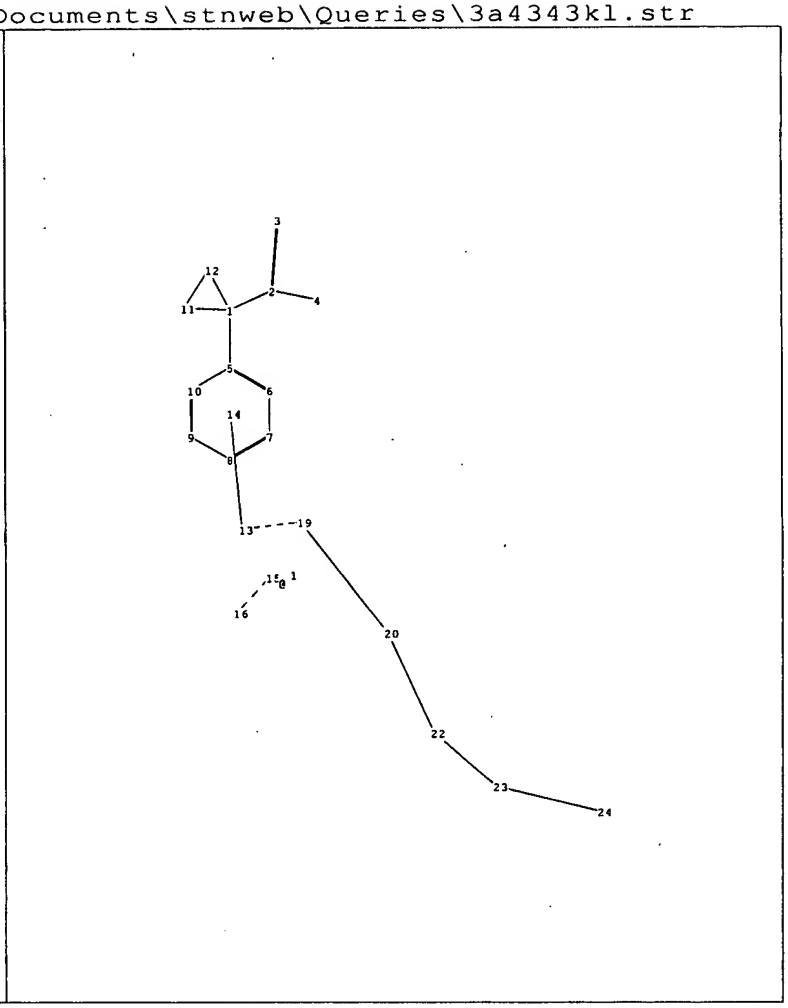
chain nodes :
2 3 4 13 15 16 19 20 22 23
ring nodes :
1 5 6 7 8 9 10 11 12 24 25 26 27 28 29 30 31 32 33
chain bonds :
1-2 1-5 2-3 2-4 13-19 15-16 19-20 20-22 22-23 23-25
ring bonds :
1-11 1-12 5-6 5-10 6-7 7-8 8-9 9-10 11-12 24-25 24-29 25-26
26-27 27-28 28-29 28-30 29-33 30-31 31-32 32-33
exact/norm bonds :
2-3 2-4 13-19 15-16 19-20 22-23 23-25 24-25 24-29 25-26 26-27
27-28
exact bonds :
1-2 1-5 1-11 1-12 11-12 20-22
normalized bonds :
5-6 5-10 6-7 7-8 8-9 9-10 28-29 28-30 29-33 30-31 31-32 32-33
isolated ring systems :
containing 1 : 5 : 24 :

G1:CH2,SO2,[*1]

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:Atom 15:CLASS 16:CLASS 19:CLASS
20:Atom 22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom
29:Atom 30:Atom 31:Atom 32:Atom 33:Atom
Element Count :
Node 20: Limited
C,C5-12

C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\3a4343kl.str





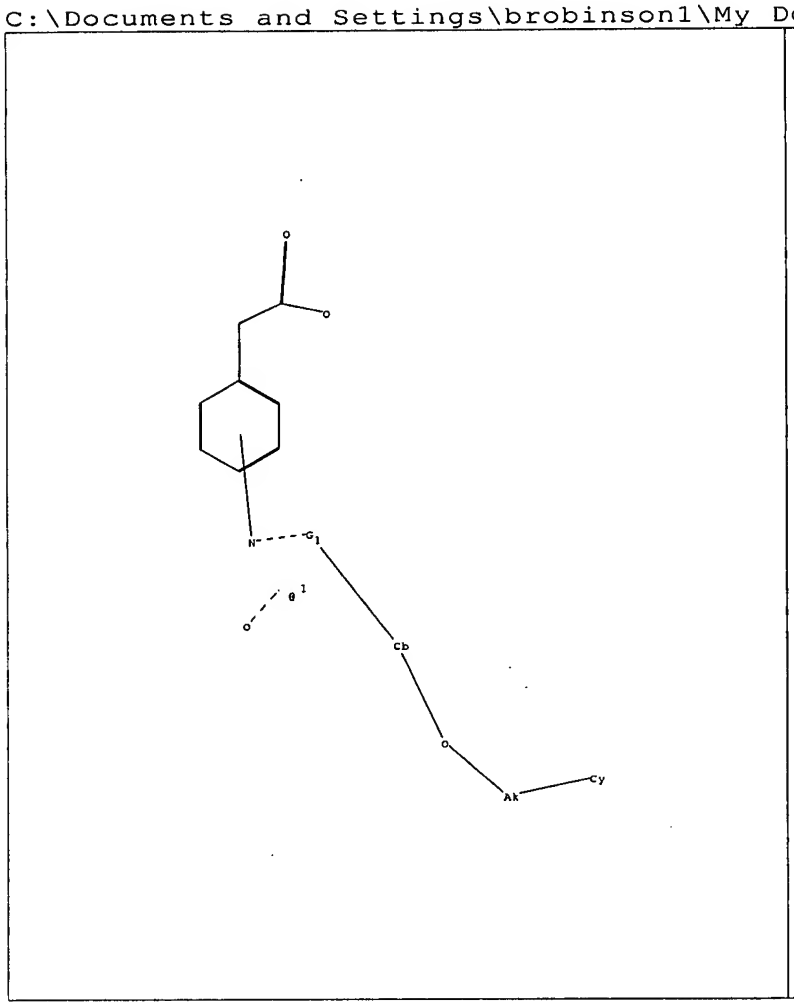
chain nodes :
2 3 4 13 15 16 19 20 22 23 24
ring nodes :
1 5 6 7 8 9 10 11 12
chain bonds :
1-2 1-5 2-3 2-4 13-19 15-16 19-20 20-22 22-23 23-24
ring bonds :
1-11 1-12 5-6 5-10 6-7 7-8 8-9 9-10 11-12
exact/norm bonds :
2-3 2-4 13-19 15-16 19-20 22-23 23-24
exact bonds :
1-2 1-5 1-11 1-12 11-12 20-22
normalized bonds :
5-6 5-10 6-7 7-8 8-9 9-10
isolated ring systems :
containing 1 : 5 :

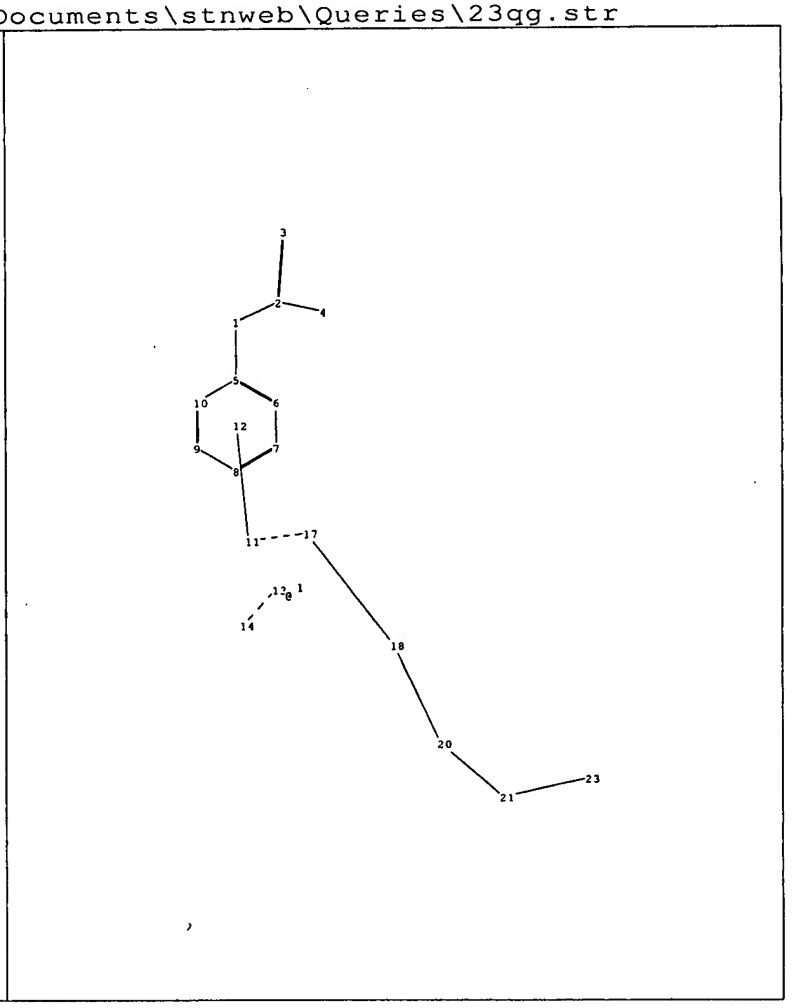
G1:CH2,SO2,[*1]

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:Atom 15:CLASS 16:CLASS 19:CLASS
20:Atom 22:CLASS 23:CLASS 24:Atom
Element Count :
Node 20: Limited
C,C5-12

Node 24: Limited
C,C7
N,N1
O,O1

C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\23qg.str





chain nodes :
1 2 3 4 11 13 14 17 18 20 21 23
ring nodes :
5 6 7 8 9 10
chain bonds :
1-2 1-5 2-3 2-4 11-17 13-14 17-18 18-20 20-21 21-23
ring bonds :
5-6 5-10 6-7 7-8 8-9 9-10
exact/norm bonds :
2-3 2-4 11-17 13-14 17-18 20-21 21-23
exact bonds :
1-2 1-5 18-20
normalized bonds :
5-6 5-10 6-7 7-8 8-9 9-10
isolated ring systems :
containing 1 : 5 :

G1:CH2,SO2,[*1]

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS 12:Atom 13:CLASS 14:CLASS 17:CLASS 18:Atom 20:CLASS
21:CLASS 23:CLASS
Element Count :
Node 18: Limited
C,C5-12

10572578

```
=> d his

     (FILE 'HOME' ENTERED AT 14:55:51 ON 06 APR 2007)

     FILE 'REGISTRY' ENTERED AT 14:56:02 ON 06 APR 2007
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           3 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 15:00:40 ON 06 APR 2007
L4           1 S L3

     FILE 'CAOLD' ENTERED AT 15:00:51 ON 06 APR 2007
L5           0 S L3

     FILE 'REGISTRY' ENTERED AT 15:00:56 ON 06 APR 2007
L6             STRUCTURE UPLOADED
L7           0 S L6
L8           0 S L6 FULL
L9             STRUCTURE UPLOADED
L10          0 S L9
L11        184 S L9 FULL

     FILE 'HCAPLUS' ENTERED AT 15:04:28 ON 06 APR 2007
L12         20 S L11
L13          1 S L12 AND NAGANAWA, A?/AU
L14         19 S L12 NOT L13
L15          1 S L14 AND IWAHASHI, M?/AU
L16          1 S L15 NOT L13
L17         18 S L14 NOT L16
L18          0 S L17 AND KINOSHITA, A?/AU
L19          0 S L17 AND SHIMABUKURO, A?/AU
L20          0 S L17 AND OGAWA, S?/AU
L21          0 S L17 AND YANO, K?/AU
L22          0 S L17 AND KOBAYASHI, K?/AU
L23          0 S L17 AND OKADA, Y?/AU
L24          0 S L17 AND KISHIDA, Y?/AU
L25          0 S L17 AND KAWAUCHI, S?/AU
L26          0 S L17 AND TSUKAMOTO, K?/AU
L27          0 S L17 AND MATSUNAGA, Y?/AU
L28          0 S L17 AND NAMBU, F?/AU

     FILE 'CAOLD' ENTERED AT 15:07:40 ON 06 APR 2007

=> s l11
L29          0 L11

=>
```

Updated Search

10572578

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1612bxr

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 4	DEC 18	CA/CAplus patent kind codes updated
NEWS 5	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 6	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS 7	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS 8	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 9	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 10	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 11	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 12	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 13	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 14	JAN 29	PHAR reloaded with new search and display fields
NEWS 15	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 17	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 18	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 19	FEB 26	MEDLINE reloaded with enhancements
NEWS 20	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 21	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 22	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 23	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 24	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 25	MAR 16	CASREACT coverage extended
NEWS 26	MAR 20	MARPAT now updated daily
NEWS 27	MAR 22	LWPI reloaded
NEWS 28	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 29	MAR 30	INPADOCDB will replace INPADOC on STN
NEWS 30	APR 02	JICST-EPLUS removed from database clusters and STN

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

Updated Search

10572578

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:55:51 ON 06 APR 2007

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:56:02 ON 06 APR 2007
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2007 HIGHEST RN 929247-80-3
DICTIONARY FILE UPDATES: 5 APR 2007 HIGHEST RN 929247-80-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\232329il.str

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 15:00:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3 TO ITERATE

100.0% PROCESSED 3 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

Updated Search

10572578

PROJECTED ITERATIONS: 3 TO 163
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:00:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 68 TO ITERATE

100.0% PROCESSED 68 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

L3 3 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	175.25	175.46

FILE 'HCAPLUS' ENTERED AT 15:00:40 ON 06 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 6 Apr 2007 VOL 146 ISS 16
FILE LAST UPDATED: 5 Apr 2007 (20070405/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3
L4 1 L3

=> d l4, ibib abs hitstr, 1

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:281799 HCAPLUS
DOCUMENT NUMBER: 142:355273
TITLE: Preparation of benzoxazine compounds containing carboxylic acid moiety as DP receptor antagonists
INVENTOR(S): Naganawa, Atsushi; Iwahashi, Maki; Kinoshita, Atsushi; Shimabukuro, Atsushi; Ogawa, Seiji; Yano, Koji; Kobayashi, Kaoru; Okada, Yutaka; Kishida, Yoko; Kawauchi, Shouji; Tsukamoto, Kohki; Matsunaga, Yoko;

Updated Search

10572578

	Nambu, Fumio
PATENT ASSIGNEE(S):	Ono Pharmaceutical Co., Ltd., Japan
SOURCE:	PCT Int. Appl., 151 pp.
	CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	Japanese
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005028455	A1	20050331	WO 2004-JP13983	20040916
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004274324	A1	20050331	AU 2004-274324	20040916
CA 2539070	A1	20050331	CA 2004-2539070	20040916
EP 1666473	A1	20060607	EP 2004-773373	20040916
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
BR 2004014487	A	20061114	BR 2004-14487	20040916
CN 1882554	A	20061220	CN 2004-80033868	20040916
NO 2006001207	A	20060619	NO 2006-1207	20060315
US 2007004716	A1	20070104	US 2006-572578	20060317
PRIORITY APPLN. INFO.:			JP 2003-325198 A	20030917
			JP 2004-101863 A	20040331
			WO 2004-JP13983 W	20040916

OTHER SOURCE(S): MARPAT 142:355273

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H, alkyl, etc.; R2 = halo, etc.; R3 = halo, etc.; R4 = H, alkyl, etc.; R5 = alkyl, etc.; R12, R13 = alkyl, etc.; W = mono- or bi-carbocyclic ring, etc.; G = alkylene having N, O, S, etc.; J = mono- or bicarbocyclic ring, mono- or biheterocyclic ring; m = 1-4; n = 0-4; i = 1-11; further details on m, n, i, R2, R3, R5 are given.] were prepared For example, acylation of 3-amino-4-fluorophenylacetic acid Me ester with compound II followed by hydrolysis using aqueous NaOH afforded compound III.

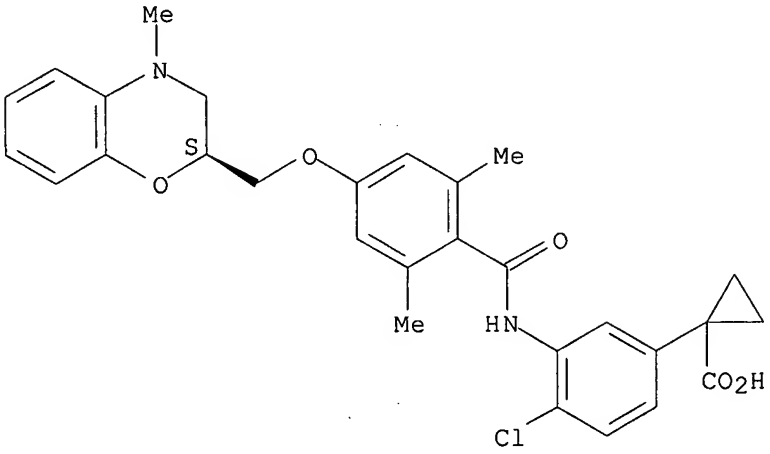
In DP (D prostanoid) receptor binding assays, compds. I exhibited the IC50 values of ≤10 μmol/L. Compds. I are claimed useful for the treatment of allergy, inflammation, etc. Formulations are given.

IT 848846-64-0P 848846-65-1P 848846-66-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoxazine compds. containing carboxylic acid moiety as DP

Updated Search

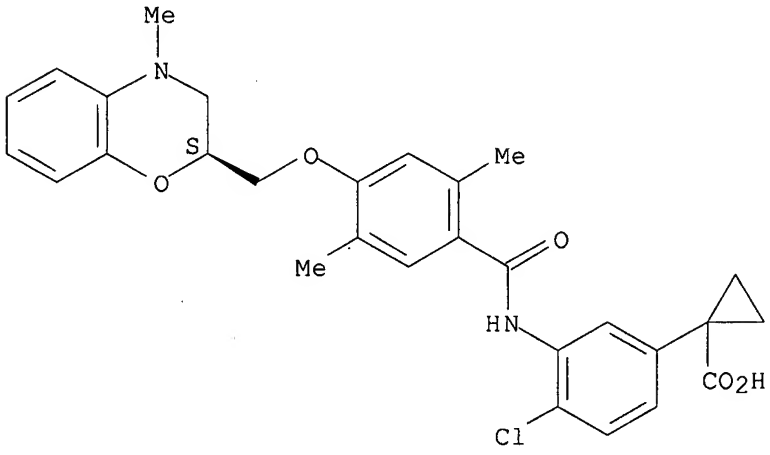
receptor antagonists for treatment of allergy, inflammation, etc.)
RN 848846-64-0 HCAPLUS
CN Cyclopropanecarboxylic acid, 1-[4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 848846-65-1 HCAPLUS
CN Cyclopropanecarboxylic acid, 1-[4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

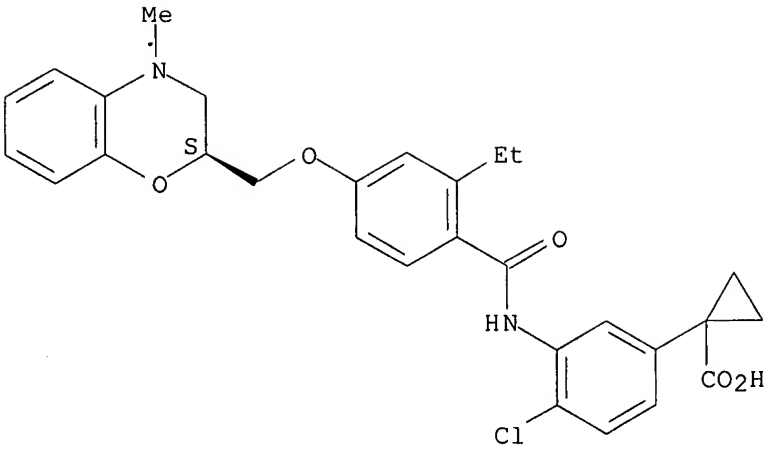


RN 848846-66-2 HCAPLUS
CN Cyclopropanecarboxylic acid, 1-[4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-ethylbenzoyl]amino]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Updated Search

10572578



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.87	183.33

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-0.78

FILE 'CAOLD' ENTERED AT 15:00:51 ON 06 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 14:55:51 ON 06 APR 2007)

FILE 'REGISTRY' ENTERED AT 14:56:02 ON 06 APR 2007
L1 STRUCTURE UPLOADED
L2 0 S L1

Updated Search

10572578

L3 3 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 15:00:40 ON 06 APR 2007
L4 1 S L3

FILE 'CAOLD' ENTERED AT 15:00:51 ON 06 APR 2007

=> s l3
L5 0 L3

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.45	183.78
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.78

FILE 'REGISTRY' ENTERED AT 15:00:56 ON 06 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 5 APR 2007 HIGHEST RN 929247-80-3
DICTIONARY FILE UPDATES: 5 APR 2007 HIGHEST RN 929247-80-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Documents and Settings\brobinson1\My
Documents\stnweb\Queries\3a4343kl.str

L6 STRUCTURE UPLOADED

=> d l6
L6 HAS NO ANSWERS
L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

Updated Search

10572578

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=> s l6
SAMPLE SEARCH INITIATED 15:02:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      139 TO ITERATE

100.0% PROCESSED      139 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         2073 TO     3487
PROJECTED ANSWERS:               0 TO        0

L7             0 SEA SSS SAM L6

=> s l6 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:02:42 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2647 TO ITERATE

100.0% PROCESSED     2647 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L8             0 SEA SSS FUL L6

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Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\23qg.str

L9      STRUCTURE UPLOADED

=> s l9
SAMPLE SEARCH INITIATED 15:04:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    29780 TO ITERATE

  6.7% PROCESSED     2000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       585280 TO   605920
PROJECTED ANSWERS:               0 TO        0

L10            0 SEA SSS SAM L9

=> s l9 full
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DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
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FULL SCREEN SEARCH COMPLETED -   597654 TO ITERATE

100.0% PROCESSED   597654 ITERATIONS                             184 ANSWERS
SEARCH TIME: 00.00.06

L11          184 SEA SSS FUL L9

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION


Updated Search
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10572578

FULL ESTIMATED COST	346.00	529.78

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.78

FILE 'HCAPLUS' ENTERED AT 15:04:28 ON 06 APR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 6 Apr 2007 VOL 146 ISS 16
FILE LAST UPDATED: 5 Apr 2007 (20070405/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s l11
L12         20 L11

=> s l12 and naganawa, a?/au
            29 NAGANAWA, A?/AU
L13          1 L12 AND NAGANAWA, A?/AU

=> d l13, ibib abs hitstr, 1
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L13 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:	2005:281799 HCAPLUS
DOCUMENT NUMBER:	142:355273
TITLE:	Preparation of benzoxazine compounds containing carboxylic acid moiety as DP receptor antagonists
INVENTOR(S):	Naganawa, Atsushi; Iwahashi, Maki; Kinoshita, Atsushi; Shimabukuro, Atsushi; Ogawa, Seiji; Yano, Koji; Kobayashi, Kaoru; Okada, Yutaka; Kishida, Yoko; Kawauchi, Shouji; Tsukamoto, Kohki; Matsunaga, Yoko; Nambu, Fumio
PATENT ASSIGNEE(S):	Ono Pharmaceutical Co., Ltd., Japan
SOURCE:	PCT Int. Appl., 151 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	Japanese
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

Updated Search

10572578

WO 2005028455	A1	20050331	WO 2004-JP13983		20040916
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
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EP 1666473	A1	20060607	EP 2004-773373		20040916
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CN 1882554	A	20061220	CN 2004-80033868		20040916
NO 2006001207	A	20060619	NO 2006-1207		20060315
US 2007004716	A1	20070104	US 2006-572578		20060317
PRIORITY APPLN. INFO.:			JP 2003-325198	A	20030917
			JP 2004-101863	A	20040331
			WO 2004-JP13983	W	20040916

OTHER SOURCE(S): MARPAT 142:355273
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H, alkyl, etc.; R2 = halo, etc.; R3 = halo, etc.; R4 = H, alkyl, etc.; R5 = alkyl, etc.; R12, R13 = alkyl, etc.; W = mono- or bi-carbocyclic ring, etc.; G = alkylene having N, O, S, etc.; J = mono- or bicarbocyclic ring, mono- or biheterocyclic ring; m = 1-4; n = 0-4; i = 1-11; further details on m, n, i, R2, R3, R5 are given.] were prepared For example, acylation of 3-amino-4-fluorophenylacetic acid Me ester with compound II followed by hydrolysis using aqueous NaOH afforded compound III.
In
DP (D prostanoid) receptor binding assays, compds. I exhibited the IC50 values of ≤10 μmol/L. Compds. I are claimed useful for the treatment of allergy, inflammation, etc. Formulations are given.

IT 848846-16-2P 848846-19-5P 848846-22-0P
848846-24-2P 848846-26-4P 848846-28-6P
848846-30-0P 848846-32-2P 848846-34-4P
848846-35-5P 848846-36-6P 848846-37-7P
848846-38-8P 848846-39-9P 848846-40-2P
848846-41-3P 848846-42-4P 848846-43-5P
848846-44-6P 848846-45-7P 848846-46-8P
848846-47-9P 848846-48-0P 848846-49-1P
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848846-53-7P 848846-54-8P 848846-55-9P
848846-56-0P 848846-57-1P 848846-58-2P
848846-59-3P 848846-60-6P 848846-61-7P
848846-62-8P 848846-63-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

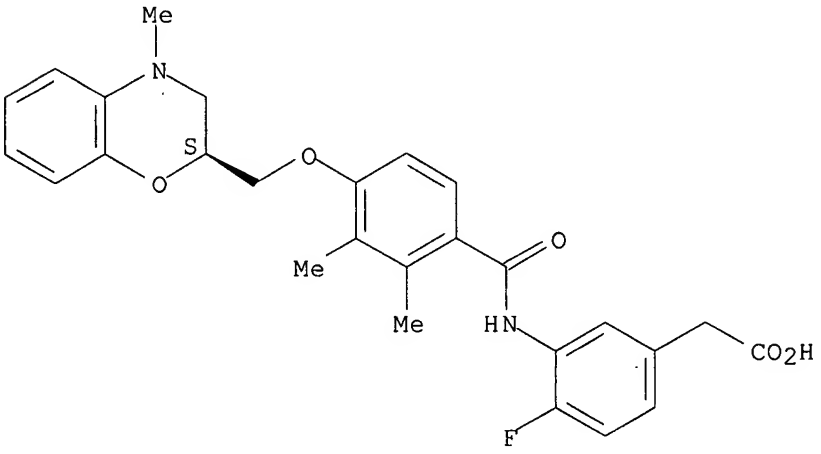
Updated Search

(preparation of benzoxazine compds. containing carboxylic acid moiety as DP receptor antagonists for treatment of allergy, inflammation, etc.)

RN 848846-16-2 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,3-dimethylbenzoyl]amino]-4-fluoro- (9CI) (CA INDEX NAME)

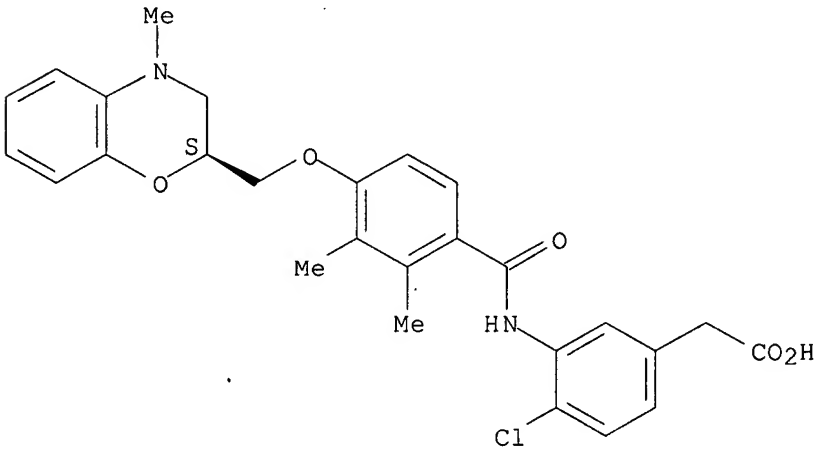
Absolute stereochemistry.



RN 848846-19-5 HCAPLUS

CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,3-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

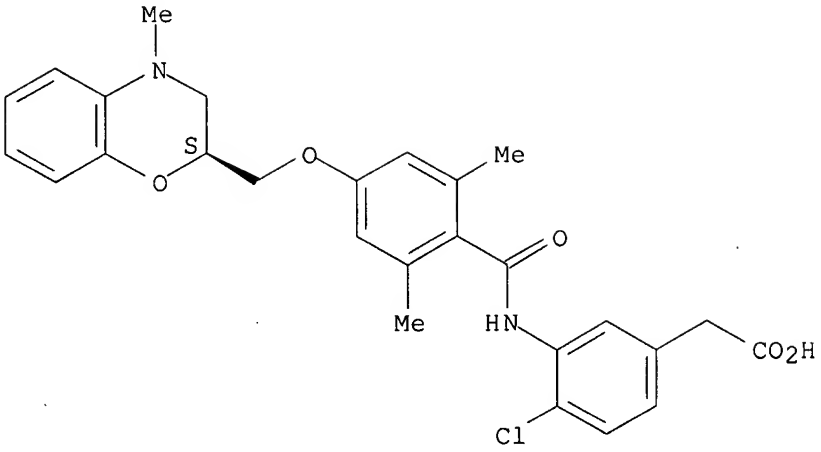


RN 848846-22-0 HCAPLUS

CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

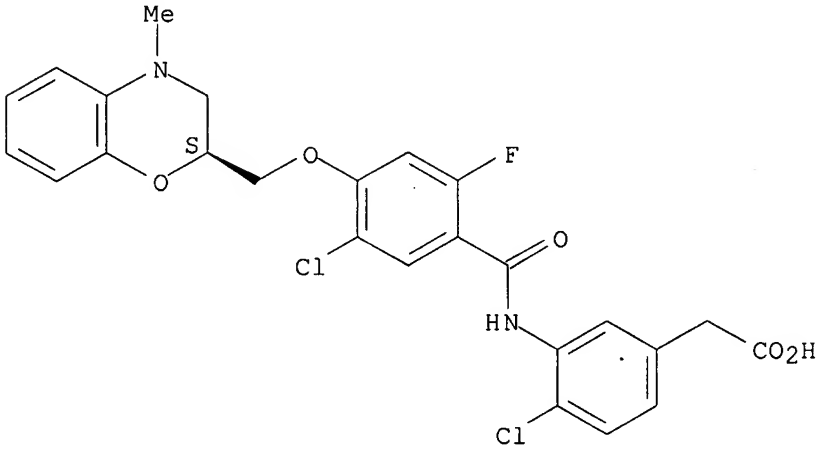
Absolute stereochemistry.

Updated Search



RN 848846-24-2 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[5-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-fluorobenzoyl]amino]- (9CI) (CA INDEX NAME)

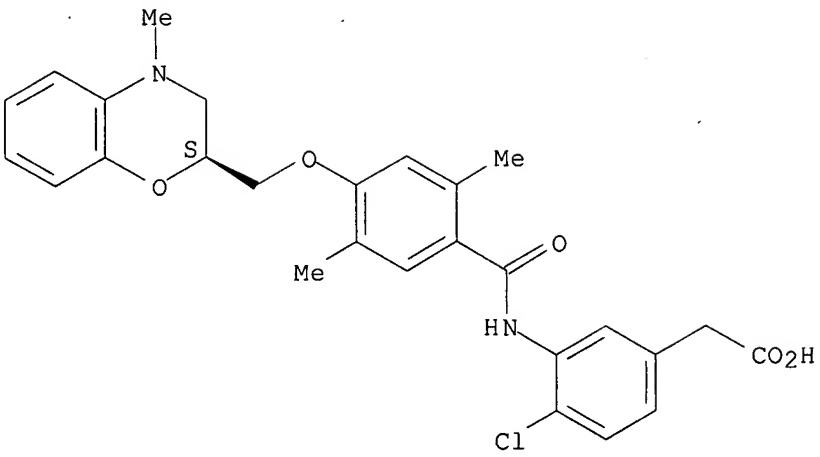
Absolute stereochemistry.



RN 848846-26-4 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

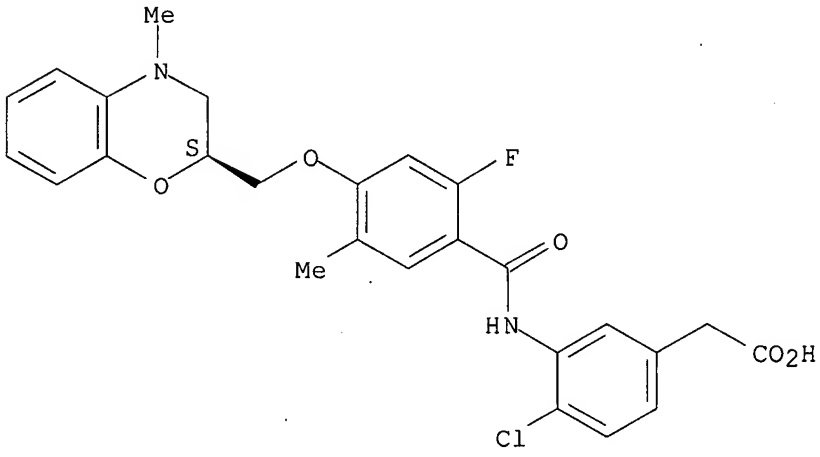
Absolute stereochemistry.

Updated Search



RN 848846-28-6 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-fluoro-5-methylbenzoyl]amino]- (9CI) (CA INDEX NAME)

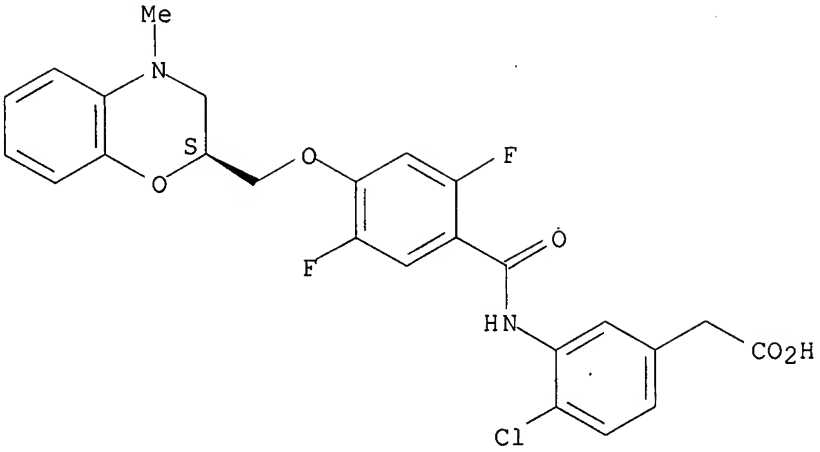
Absolute stereochemistry.



RN 848846-30-0 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-difluorobenzoyl]amino]- (9CI) (CA INDEX NAME)

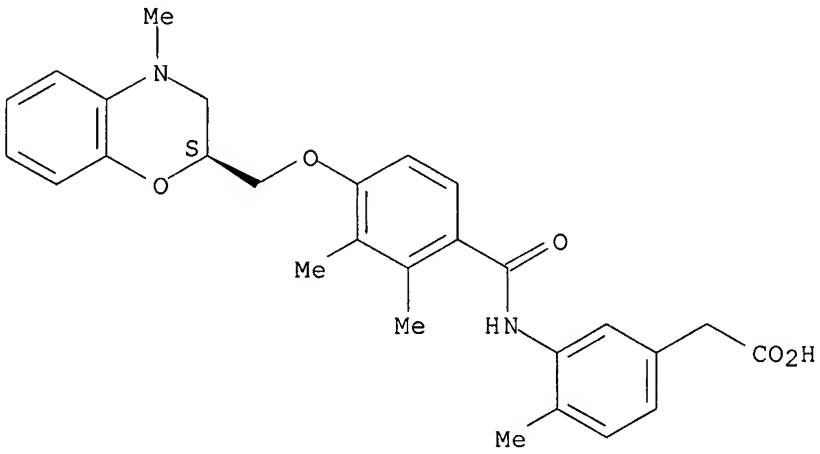
Absolute stereochemistry.

Updated Search



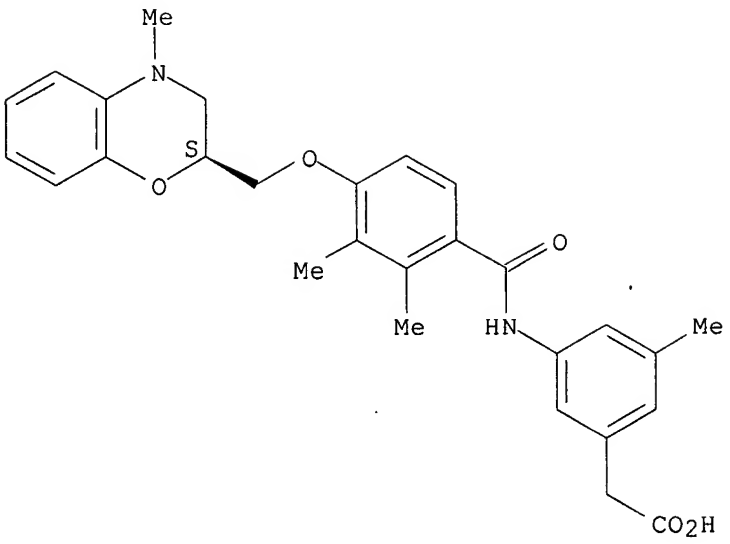
RN 848846-32-2 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,3-dimethylbenzoyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



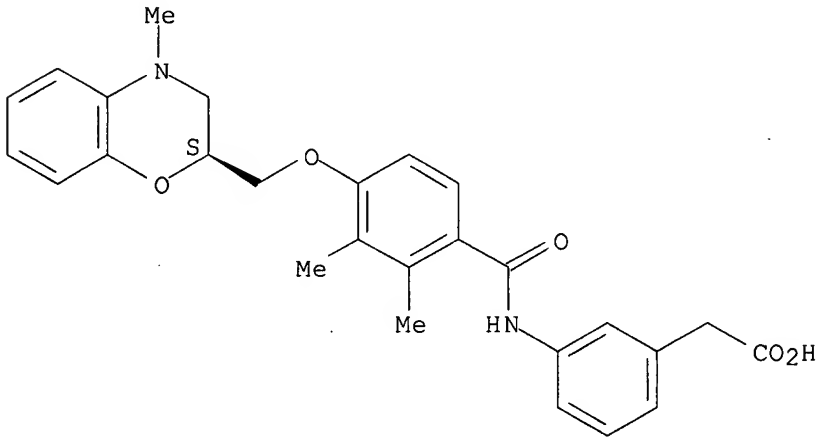
RN 848846-34-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,3-dimethylbenzoyl]amino]-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 848846-35-5 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,3-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

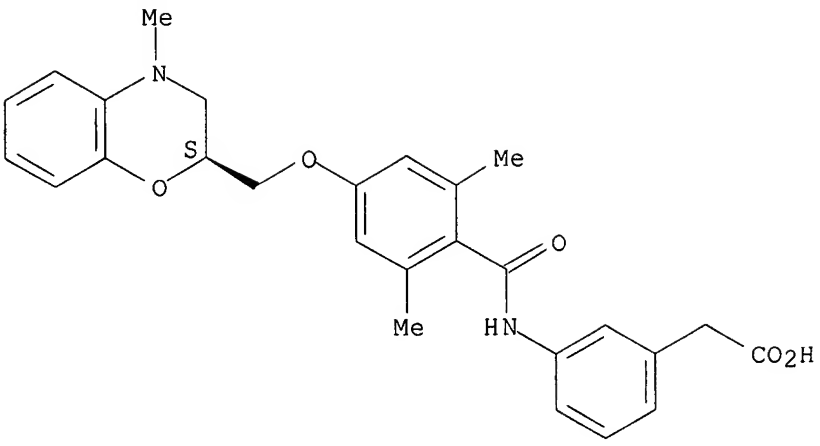
Absolute stereochemistry.



RN 848846-36-6 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

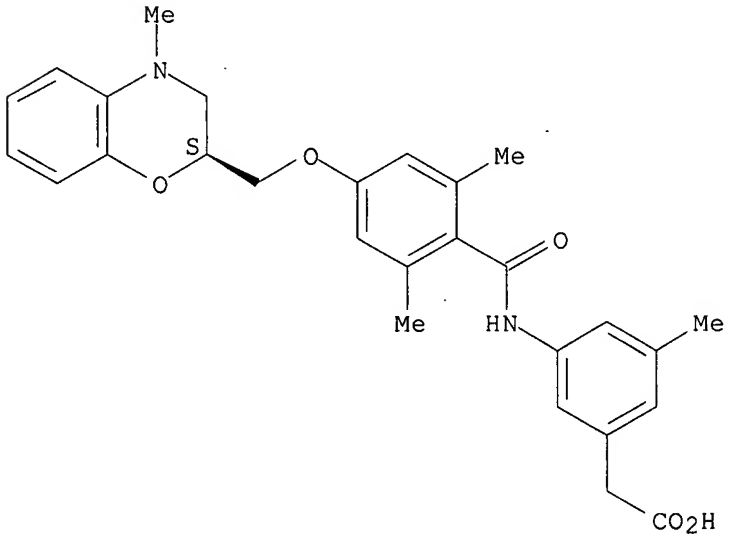
Absolute stereochemistry.

Updated Search



RN 848846-37-7 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]-5-methyl- (9CI) (CA INDEX NAME)

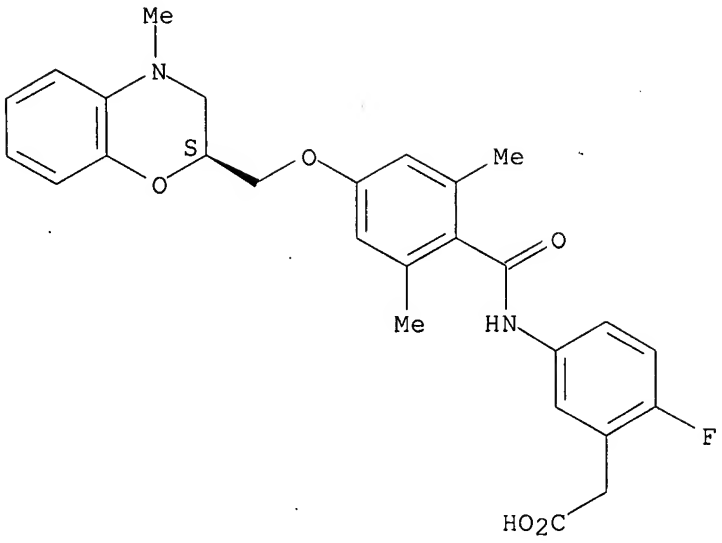
Absolute stereochemistry.



RN 848846-38-8 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]-2-fluoro- (9CI) (CA INDEX NAME)

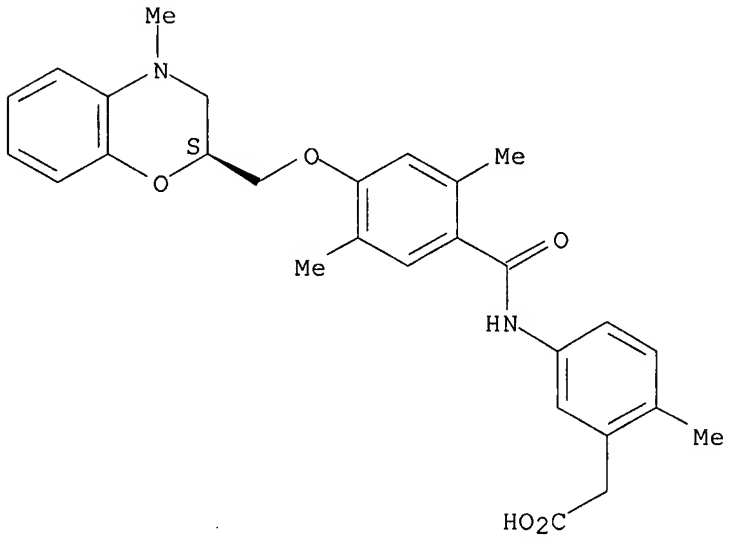
Absolute stereochemistry.

Updated Search



RN 848846-39-9 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

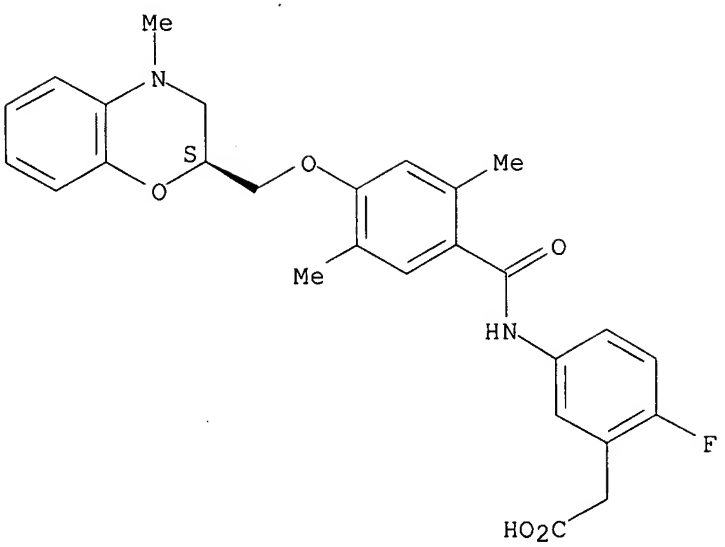
Absolute stereochemistry.



RN 848846-40-2 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]-2-fluoro- (9CI) (CA INDEX NAME)

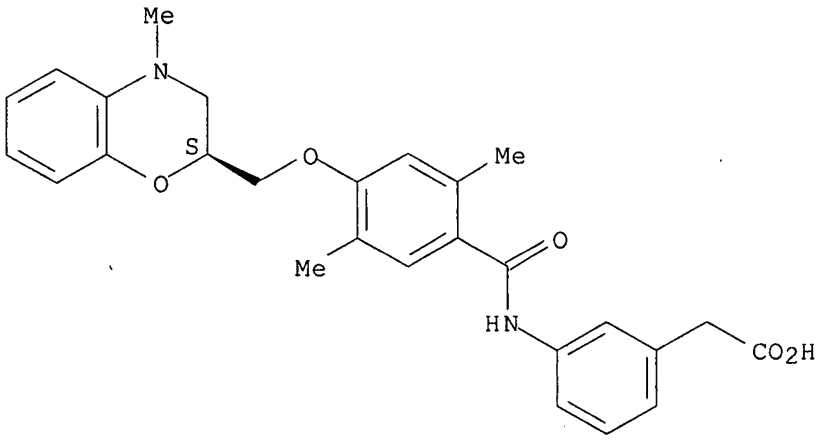
Absolute stereochemistry.

Updated Search



RN 848846-41-3 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

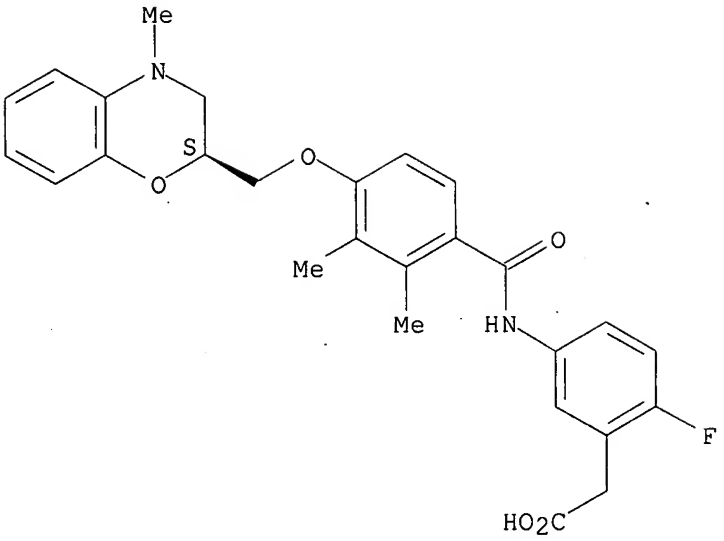
Absolute stereochemistry.



RN 848846-42-4 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,3-dimethylbenzoyl]amino]-2-fluoro- (9CI) (CA INDEX NAME)

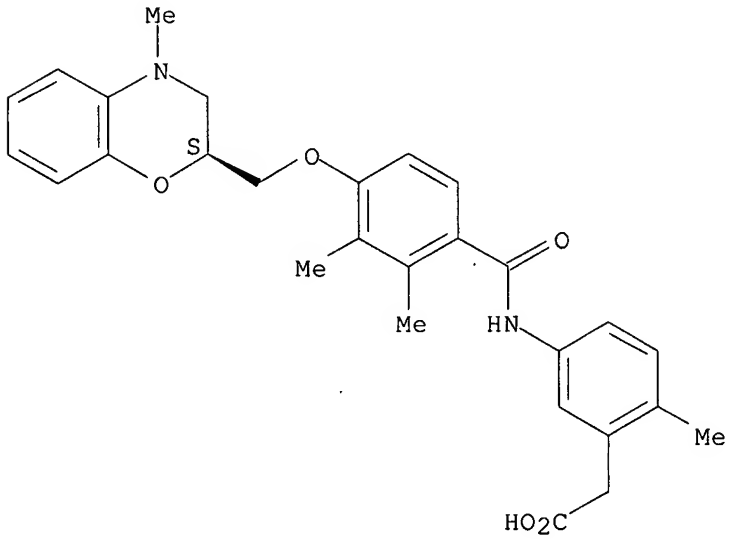
Absolute stereochemistry.

Updated Search



RN 848846-43-5 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,3-dimethylbenzoyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

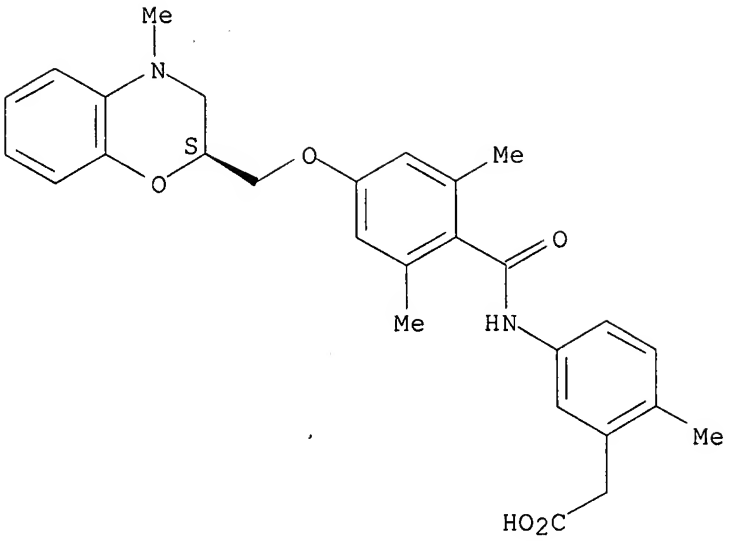
Absolute stereochemistry.



RN 848846-44-6 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

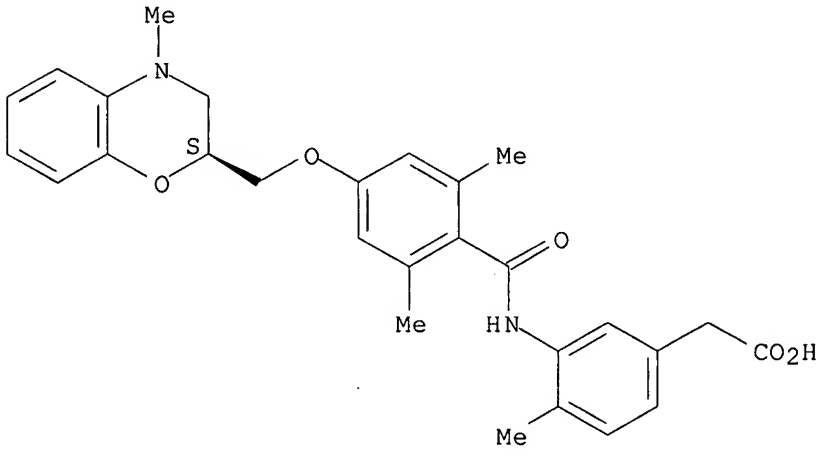
Absolute stereochemistry.

Updated Search



RN 848846-45-7 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

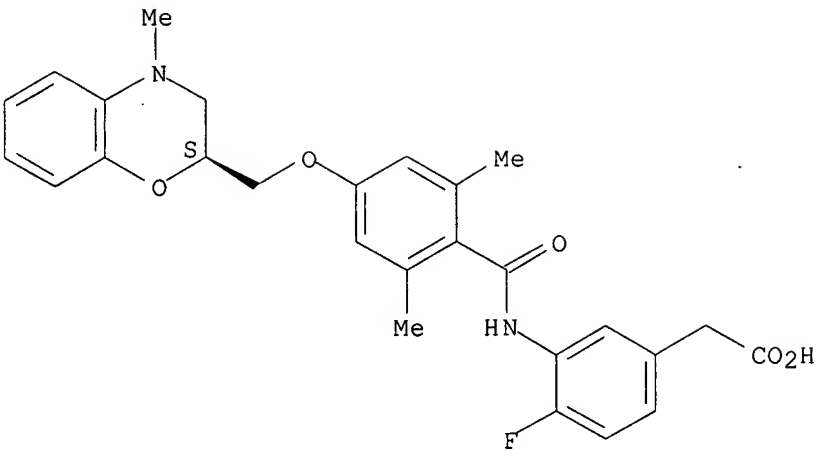
Absolute stereochemistry.



RN 848846-46-8 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]-4-fluoro- (9CI) (CA INDEX NAME)

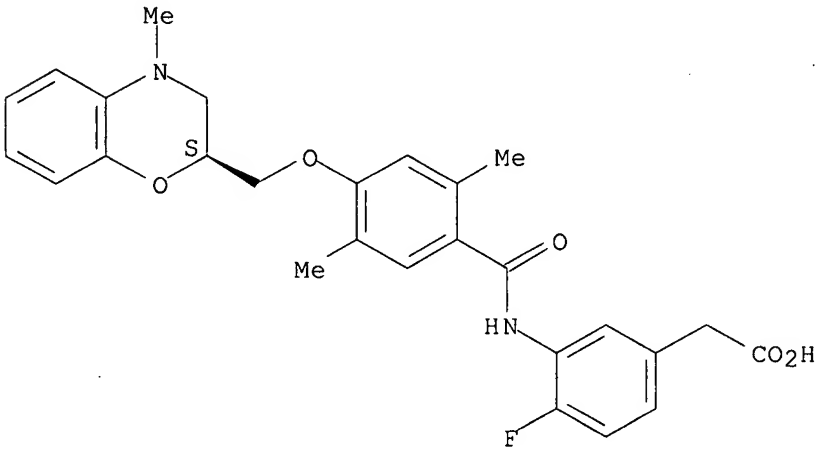
Absolute stereochemistry.

Updated Search



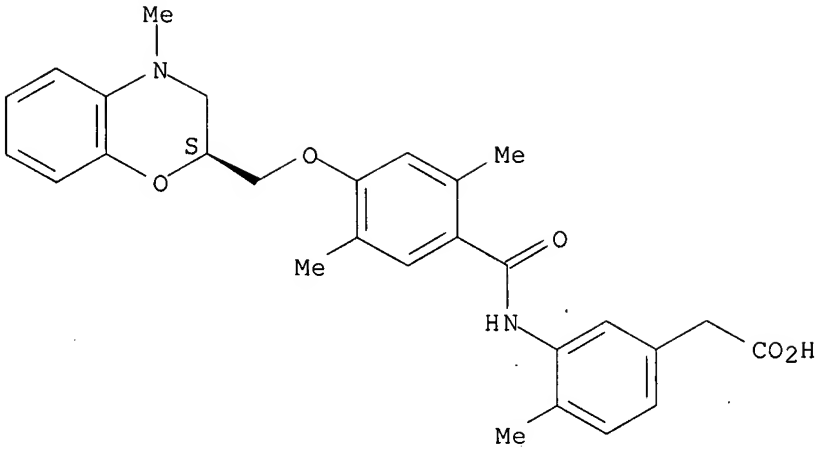
RN 848846-47-9 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]-4-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



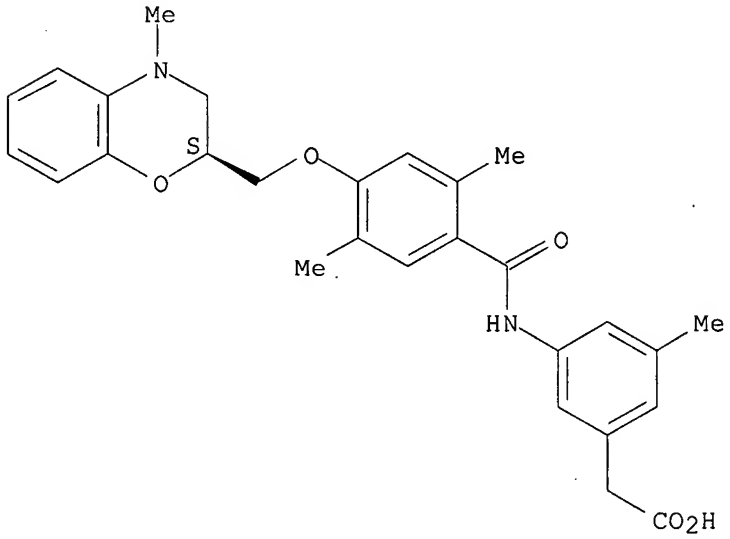
RN 848846-48-0 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 848846-49-1 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]-5-methyl- (9CI) (CA INDEX NAME)

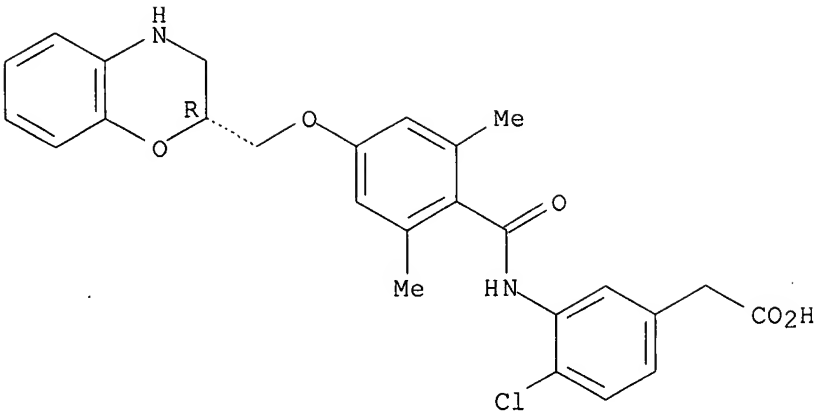
Absolute stereochemistry.



RN 848846-50-4 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2R)-3,4-dihydro-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

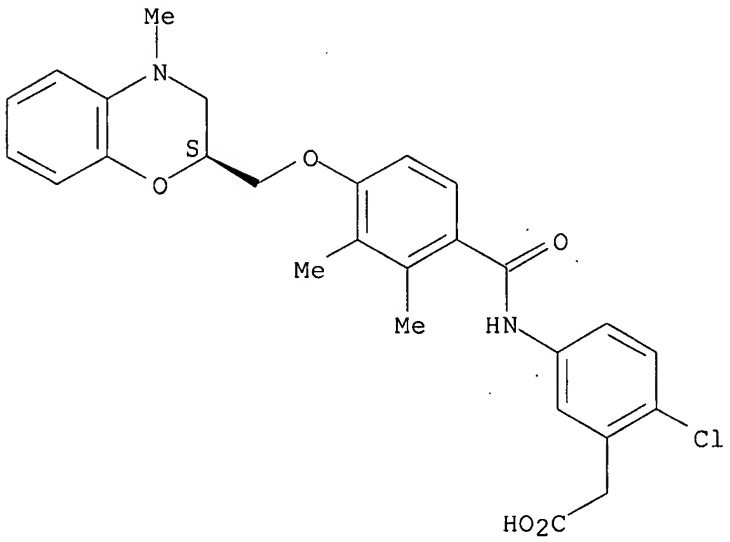
Absolute stereochemistry.

Updated Search



RN 848846-51-5 HCAPLUS
CN Benzeneacetic acid, 2-chloro-5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,3-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

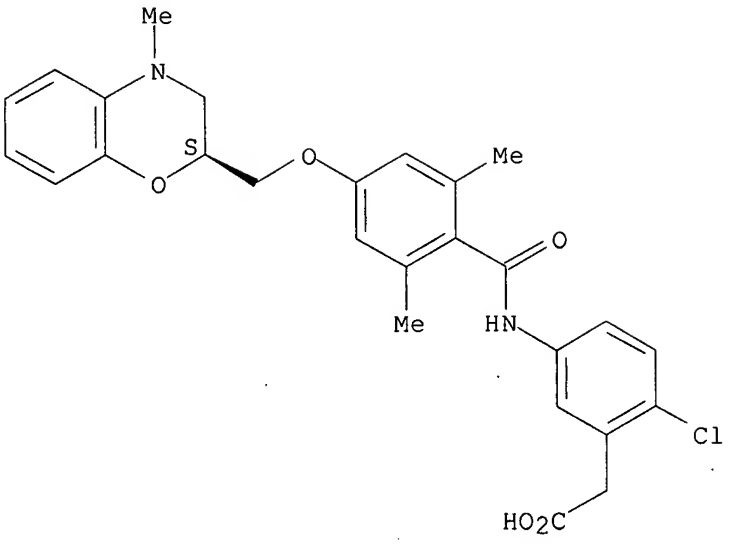
Absolute stereochemistry.



RN 848846-52-6 HCAPLUS
CN Benzeneacetic acid, 2-chloro-5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

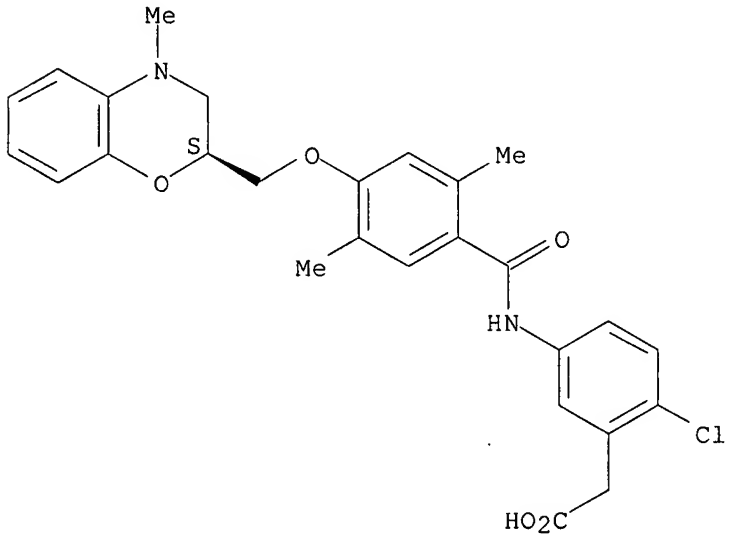
Absolute stereochemistry.

Updated Search



RN 848846-53-7 HCAPLUS
CN Benzeneacetic acid, 2-chloro-5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

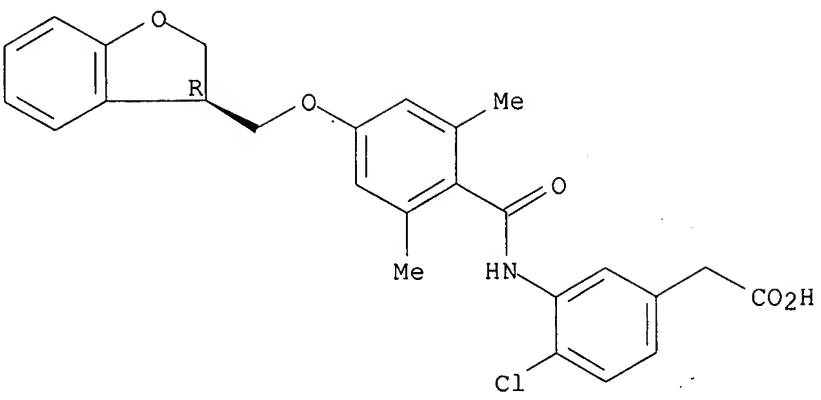
Absolute stereochemistry.



RN 848846-54-8 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(3R)-2,3-dihydro-3-benzofuranyl]methoxy]-2,6-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

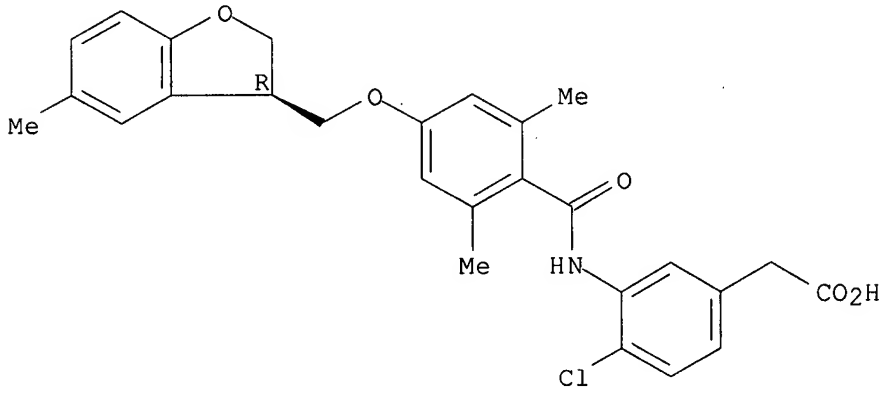
Absolute stereochemistry.

Updated Search



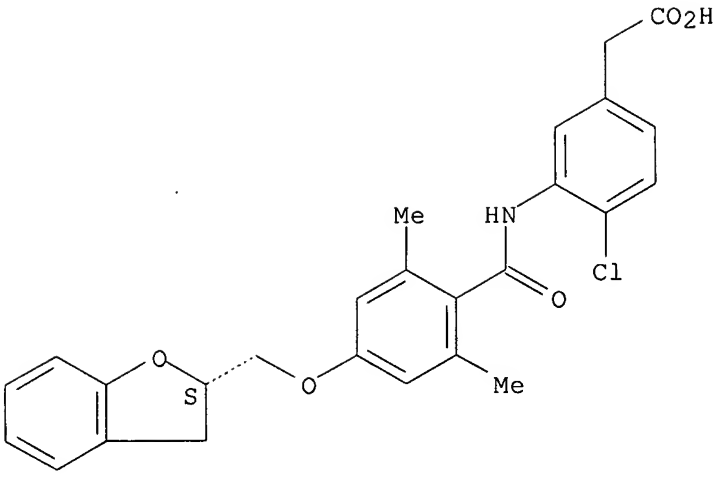
RN 848846-55-9 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(3R)-2,3-dihydro-5-methyl-3-benzofuranyl]methoxy]-2,6-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

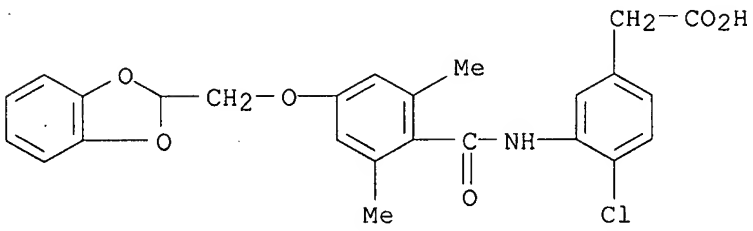


RN 848846-56-0 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-2,3-dihydro-2-benzofuranyl]methoxy]-2,6-dimethylbenzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

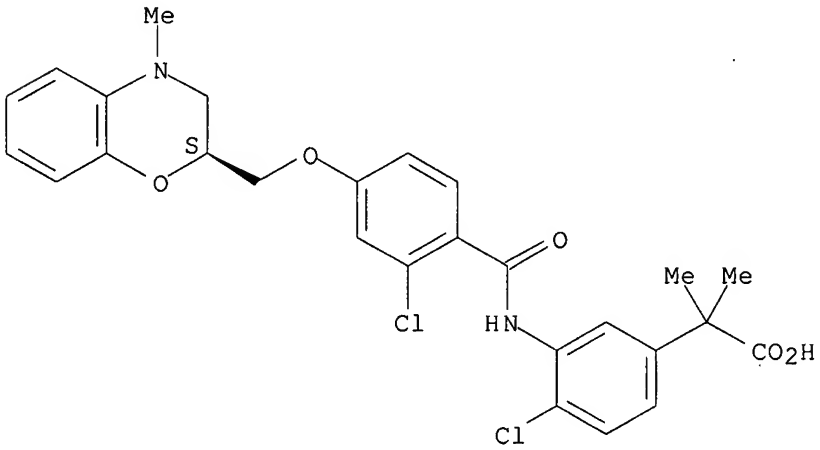


RN 848846-57-1 HCAPLUS
CN Benzeneacetic acid, 3-[[4-(1,3-benzodioxol-2-ylmethoxy)-2,6-dimethylbenzoyl]amino]-4-chloro- (9CI) (CA INDEX NAME)



RN 848846-58-2 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α,α-dimethyl- (9CI) (CA INDEX NAME)

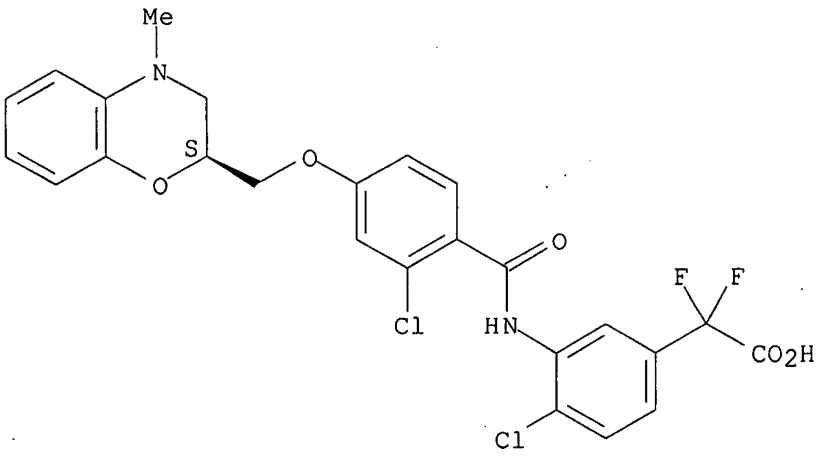
Absolute stereochemistry.



Updated Search

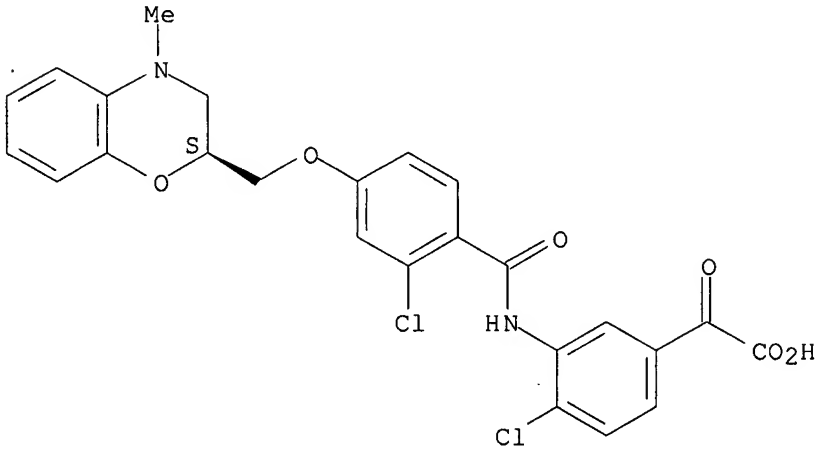
RN 848846-59-3 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α,α-difluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 848846-60-6 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α-oxo- (9CI) (CA INDEX NAME)

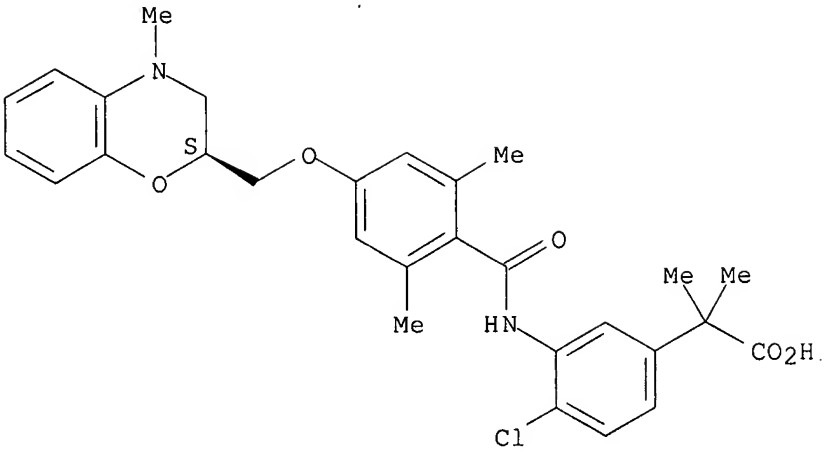
Absolute stereochemistry.



RN 848846-61-7 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]-α,α-dimethyl- (9CI) (CA INDEX NAME)

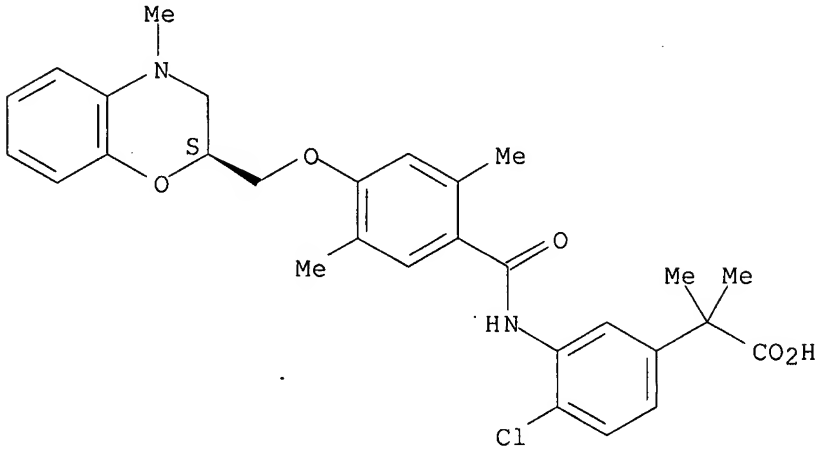
Absolute stereochemistry.

Updated Search



RN 848846-62-8 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]-α,α-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 848846-63-9 HCAPLUS
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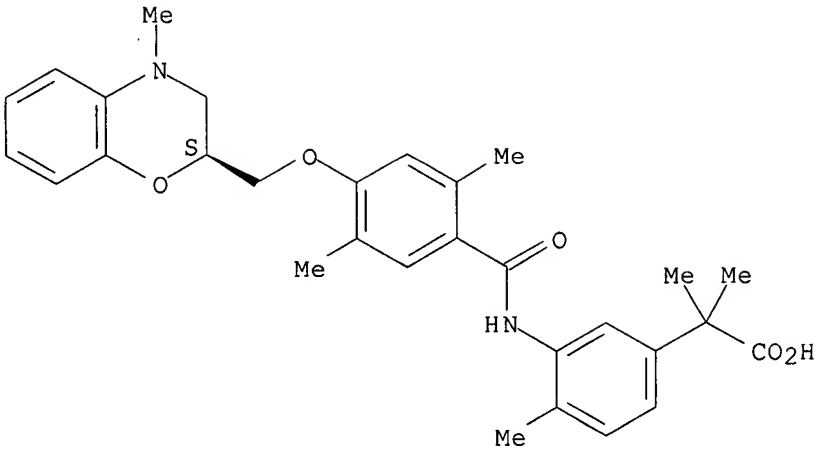
Absolute stereochemistry.

Updated Search

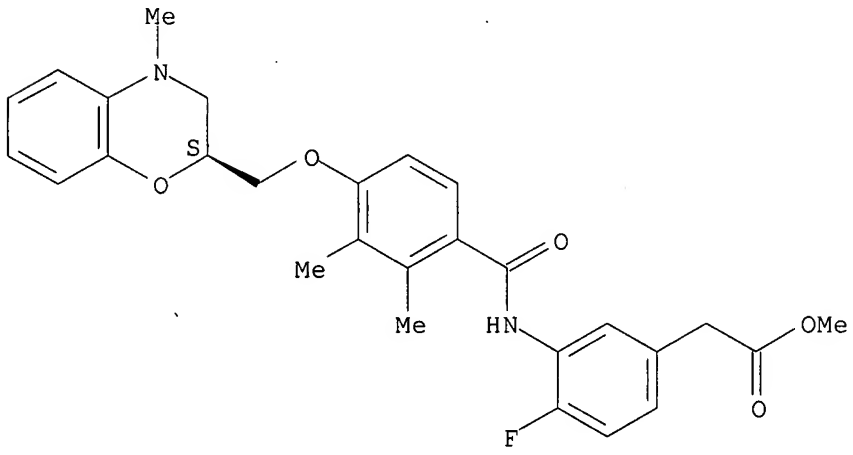


IT 848846-70-8P 848846-73-1P 848846-78-6P
848846-81-1P 848846-82-2P 848846-83-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzoxazine compds. containing carboxylic acid moiety as DP receptor antagonists for treatment of allergy, inflammation, etc.)

RN 848846-70-8 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,3-dimethylbenzoyl]amino]-4-fluoro-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

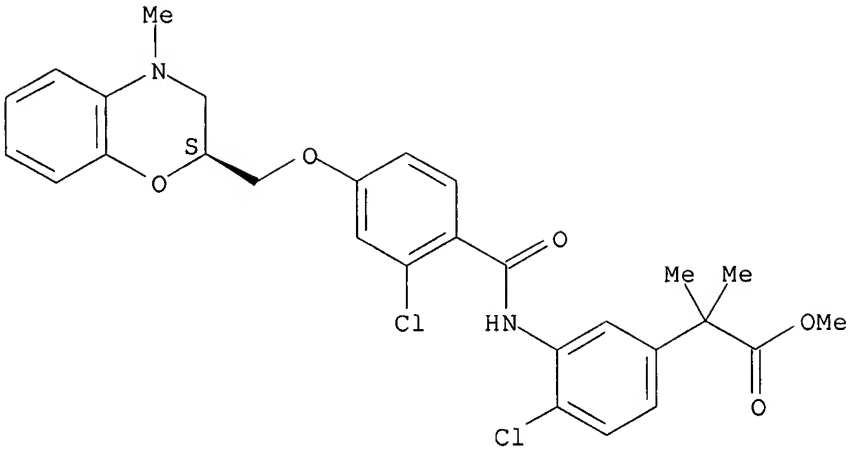


RN 848846-73-1 HCAPLUS

CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α,α-dimethyl-, methyl ester (9CI) (CA INDEX NAME)

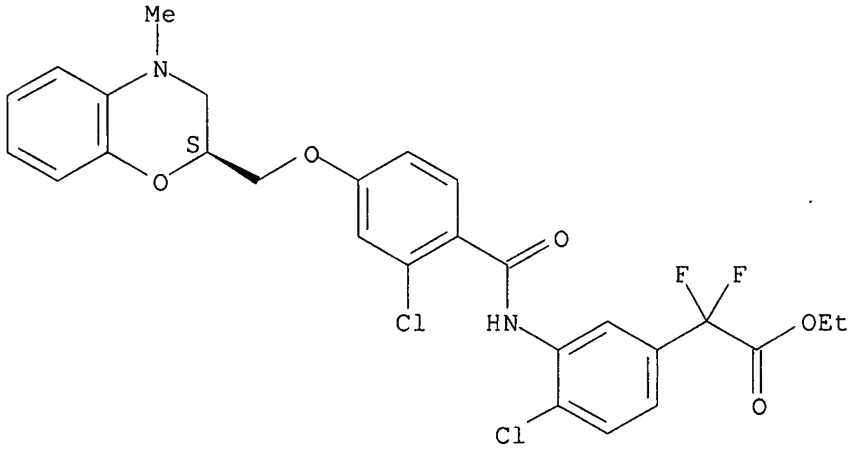
Absolute stereochemistry.

Updated Search



RN 848846-78-6 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α,α-difluoro-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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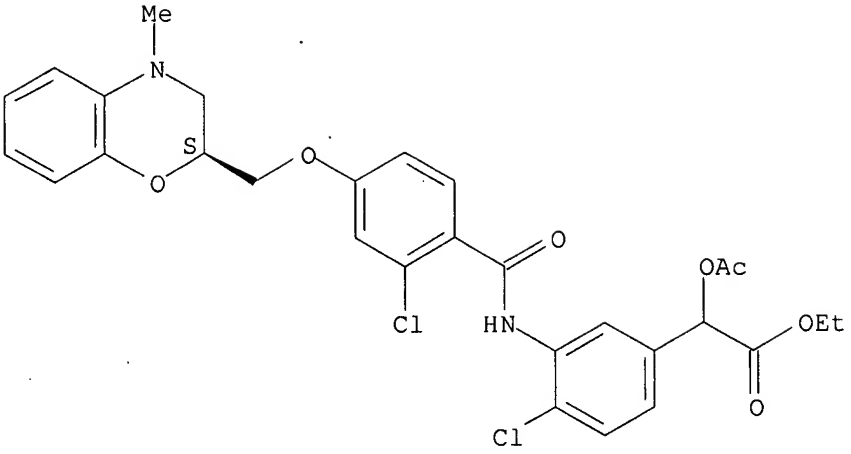
CN Benzeneacetic acid, α-(acetyloxy)-4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

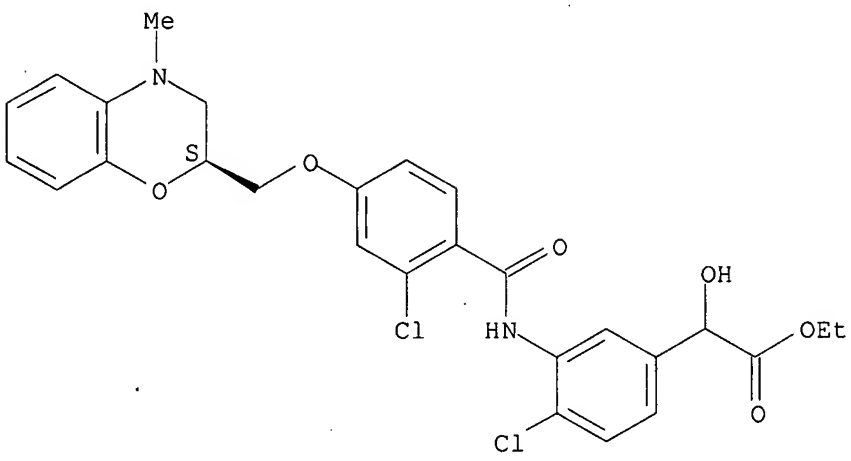
Absolute stereochemistry.

Updated Search



RN 848846-82-2 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

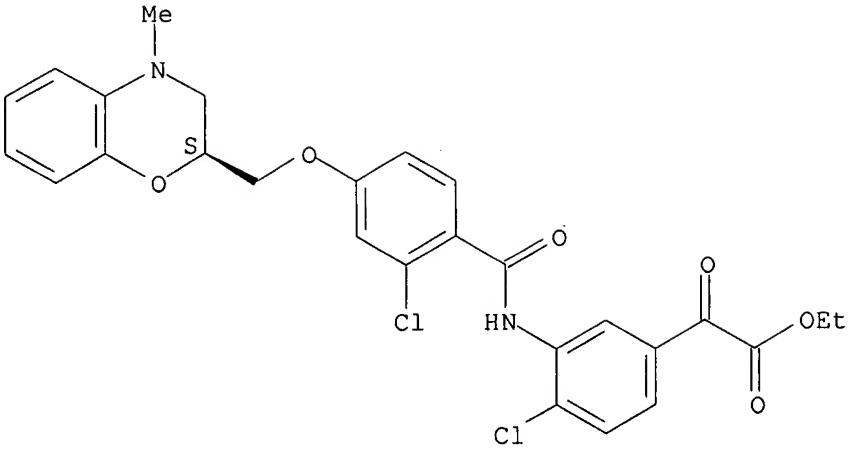


RN 848846-83-3 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α-oxo-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Updated Search

10572578



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'HCAPLUS' ENTERED AT 15:00:40 ON 06 APR 2007
L4 1 S L3

FILE 'CAOLD' ENTERED AT 15:00:51 ON 06 APR 2007
L5 0 S L3

FILE 'REGISTRY' ENTERED AT 15:00:56 ON 06 APR 2007
L6 STRUCTURE UPLOADED
L7 0 S L6
L8 0 S L6 FULL
L9 STRUCTURE UPLOADED
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L11 184 S L9 FULL

FILE 'HCAPLUS' ENTERED AT 15:04:28 ON 06 APR 2007
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L15 1 L14 AND IWAHASHI, M?/AU

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L16 1 L15 NOT L13

Updated Search

10572578

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L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN
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DOCUMENT NUMBER: 139:261306
TITLE: Preparation of 3-[4-[(2S)-4-methyl-3,4-dihydro-2H-1,4-benzoxazin-2-ylmethoxy]benzoylamino]phenylacetic acid derivatives as prostaglandin DP receptor antagonists
INVENTOR(S): Iwahashi, Maki; Kobayashi, Kaoru; Nambu, Fumio
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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EP 1486491	A1	20041215	EP 2003-710260	20030306
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CN 1656085	A	20050817	CN 2003-811495	20030306
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NO 2004003894	A	20041217	NO 2004-3894	20040917
US 2005222216	A1	20051006	US 2005-507885	20050517
PRIORITY APPLN. INFO.:			JP 2002-76456 A	20020319
			WO 2003-JP2635 W	20030306

OTHER SOURCE(S): MARPAT 139:261306
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title benzoxazine derivs. with general formula of I [wherein R1 = H, alkyl, alkenyl, or PhCH2; E = CO, SO2, or CH2; R2 and R3 = independently halo, alkoxy, OH, trihalomethyl, CN, Ph, Py, NO2, or (un)substituted alkyl; R4 = H, alkyl, or PhCH2; R5 = alkoxy, halo, OH, trihalomethyl, NO2, Ph, PhO, oxo, acyl, CN, (un)substituted alkyl, amino, or SO2H; ring W and ring J = independently (hetero)cyclohydrocarbyl; G = alkylene, alkenylene, or alkynylene, etc.; m = 0-4; n = 0-4; p = 0-11; etc.] are prepared as

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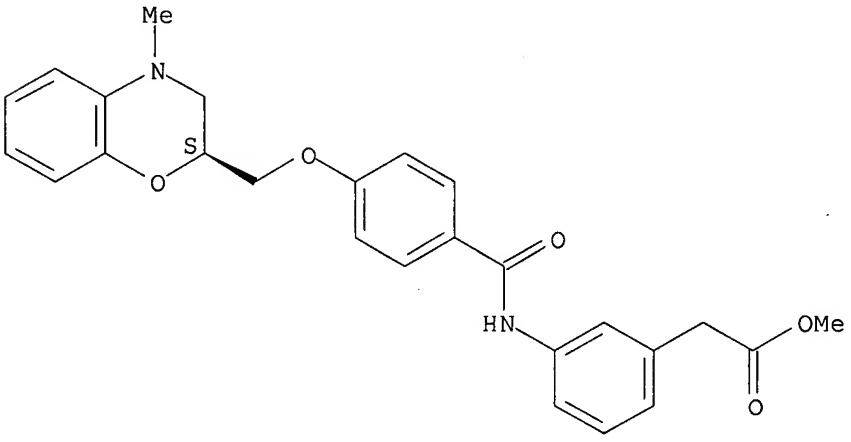
prostaglandin DP receptor antagonists. I are useful in preventing and/or treating allergic diseases (allergic nephritis, allergic conjunctivitis, atopic dermatitis, bronchial asthma, food allergy, etc.), systemic mast cell disease, systemic mast cell activation failure, anaphylactic shock, respiratory tract contraction, urticaria, eczema, diseases associated with itch (atopic dermatitis, urticaria, etc.), diseases (cataract, retinal detachment, inflammation, infection, sleep disorder, etc.) secondarily caused by behaviors associating itch (scratching, beating, etc.), inflammation, chronic obstructive pulmonary disease, ischemic reperfusion injury, cerebrovascular disorder, rheumatoid arthritis, pleuritis, ulcerative colitis, and so on (no data). For example, 3-aminophenylacetic acid Me ester (preparation given) was reacted with 4-[(2S)-4-methyl-3,4-dihydro-2H-1,4-benzoxazin-2-ylmethoxy]benzoyl chloride (preparation given) in Ch2Cl2 in the presence of pyridine to give II. I showed affinity towards prostaglandin DP receptor with Ki of <10 μM in guinea pig. Formulations containing I as an active ingredient were also described.

IT 603107-22-8P 603107-23-9P 603107-24-0P
603107-25-1P 603107-26-2P 603107-27-3P
603107-28-4P 603107-29-5P 603107-30-8P
603107-31-9P 603107-32-0P 603107-33-1P
603107-34-2P 603107-35-3P 603107-36-4P
603107-37-5P 603107-54-6P 603107-55-7P
603107-58-0P 603107-60-4P 603107-61-5P
603107-63-7P 603107-64-8P 603107-65-9P
603107-66-0P 603107-67-1P 603107-68-2P
603107-69-3P 603107-70-6P 603107-71-7P
603107-72-8P 603107-73-9P 603107-74-0P
603108-03-8P 603108-05-0P 603108-11-8P
603108-13-0P 603108-15-2P 603108-17-4P
603108-18-5P 603108-20-9P 603108-34-5P
603108-49-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of aminophenylacetic acid derivs. as prostaglandin DP receptor antagonists)

RN 603107-22-8 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

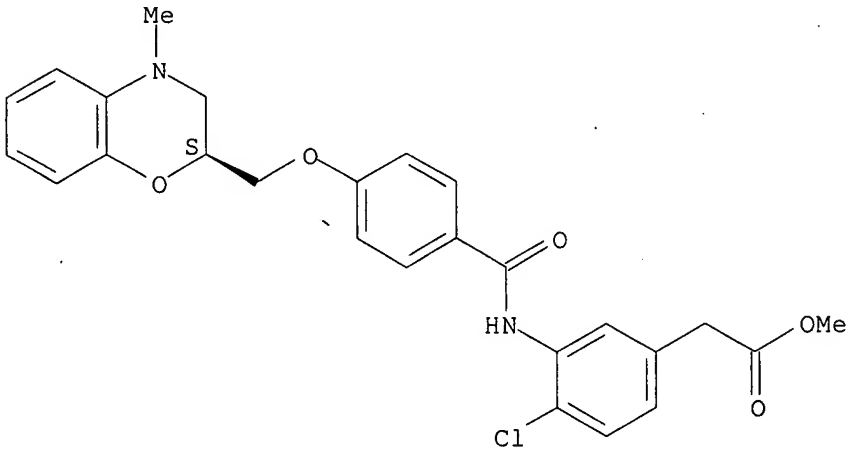
Absolute stereochemistry.



Updated Search

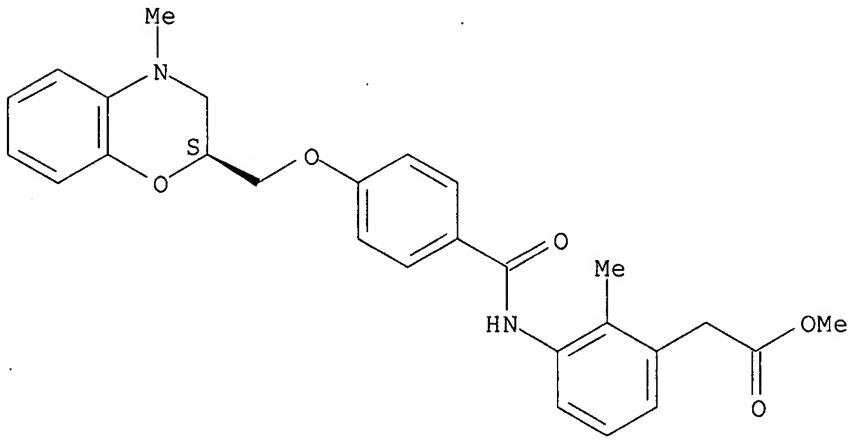
RN 603107-23-9 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 603107-24-0 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)

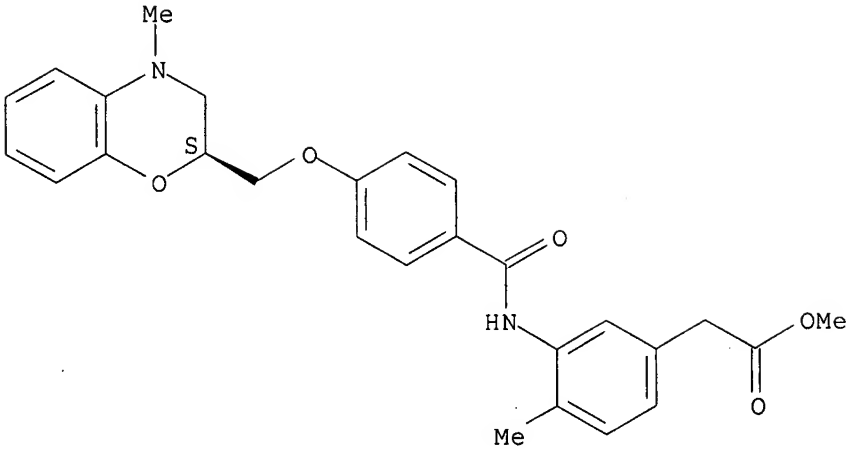
Absolute stereochemistry.



RN 603107-25-1 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-methyl-, methyl ester (9CI) (CA INDEX NAME)

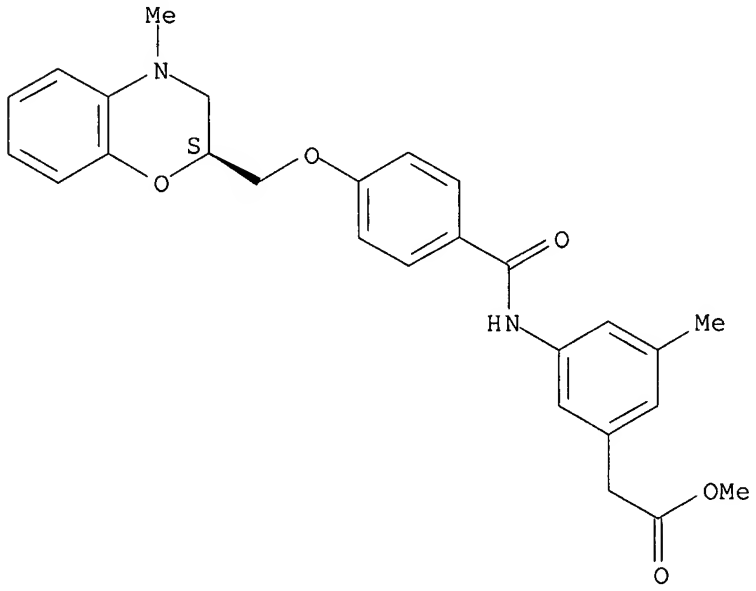
Absolute stereochemistry.

Updated Search



RN 603107-26-2 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-5-methyl-, methyl ester (9CI) (CA INDEX NAME)

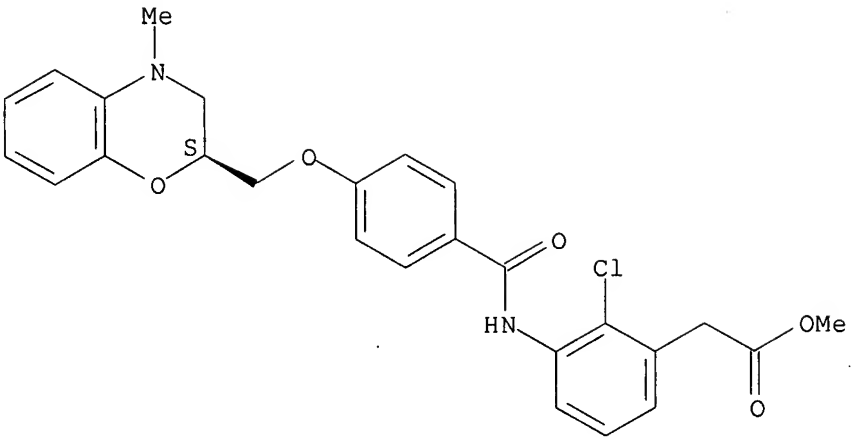
Absolute stereochemistry.



RN 603107-27-3 HCAPLUS
CN Benzeneacetic acid, 2-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

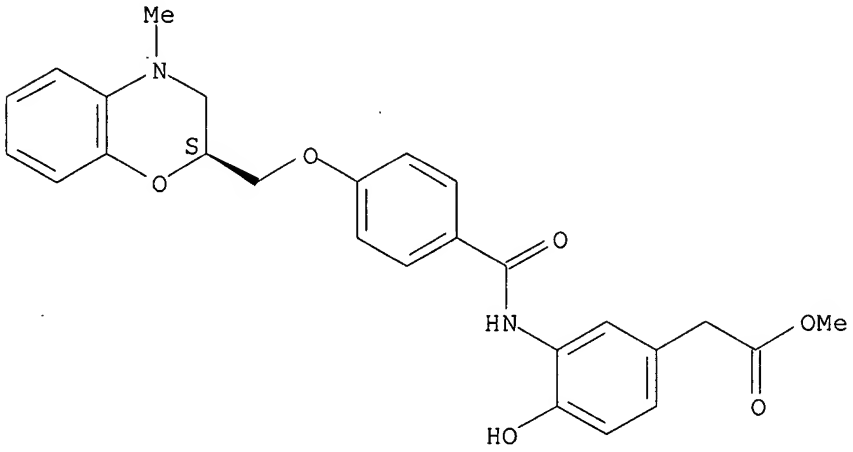
Absolute stereochemistry.

Updated Search



RN 603107-28-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)

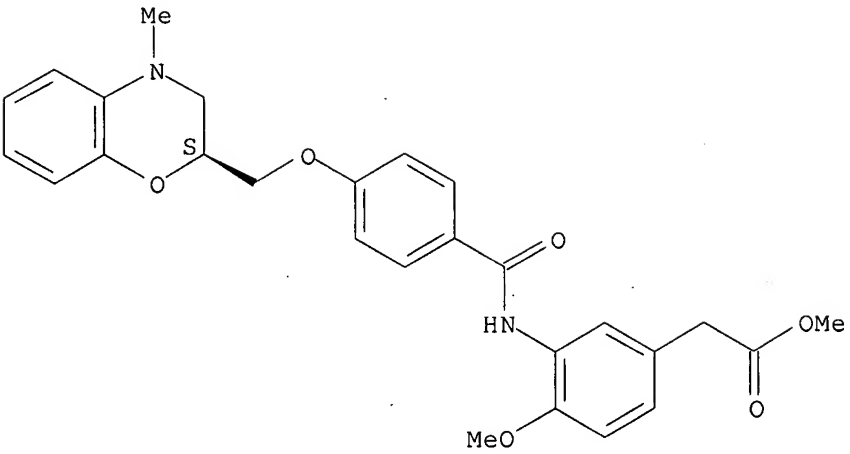
Absolute stereochemistry.



RN 603107-29-5 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-methoxy-, methyl ester (9CI) (CA INDEX NAME)

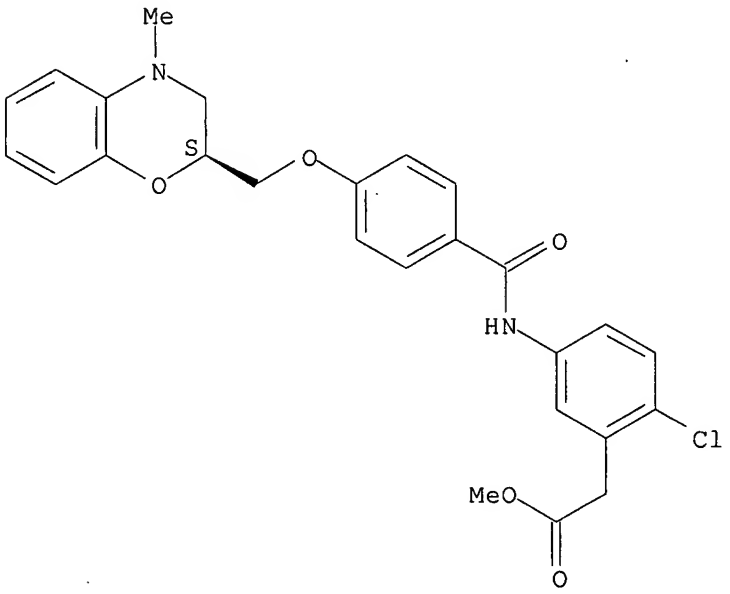
Absolute stereochemistry.

Updated Search



RN 603107-30-8 HCAPLUS
CN Benzeneacetic acid, 2-chloro-5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

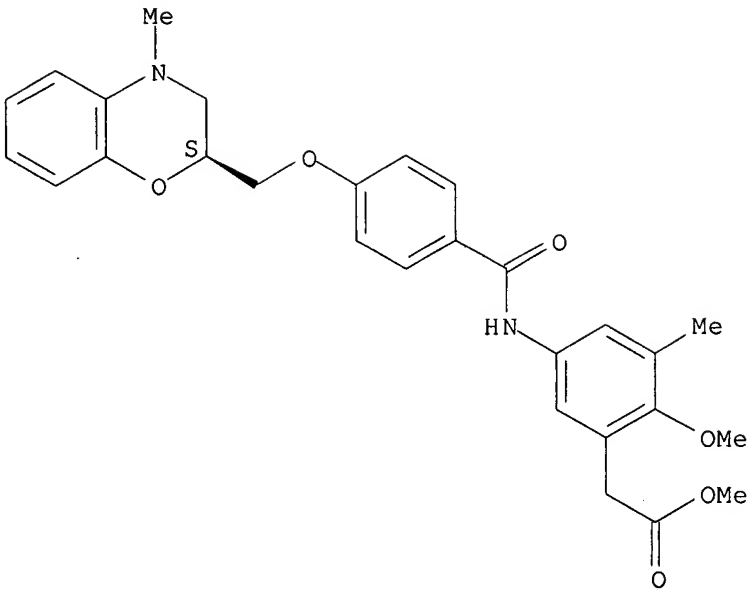
Absolute stereochemistry.



RN 603107-31-9 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methoxy-3-methyl-, methyl ester (9CI) (CA INDEX NAME)

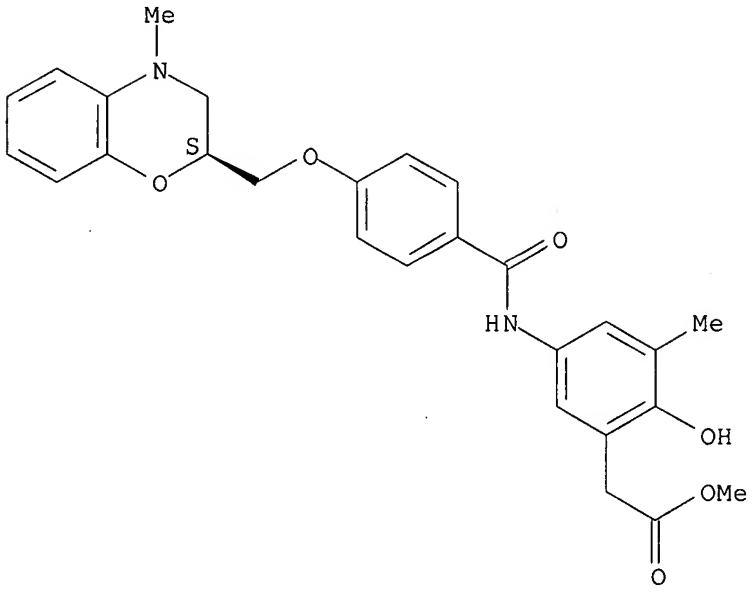
Absolute stereochemistry.

Updated Search



RN 603107-32-0 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-hydroxy-3-methyl-, methyl ester (9CI) (CA INDEX NAME)

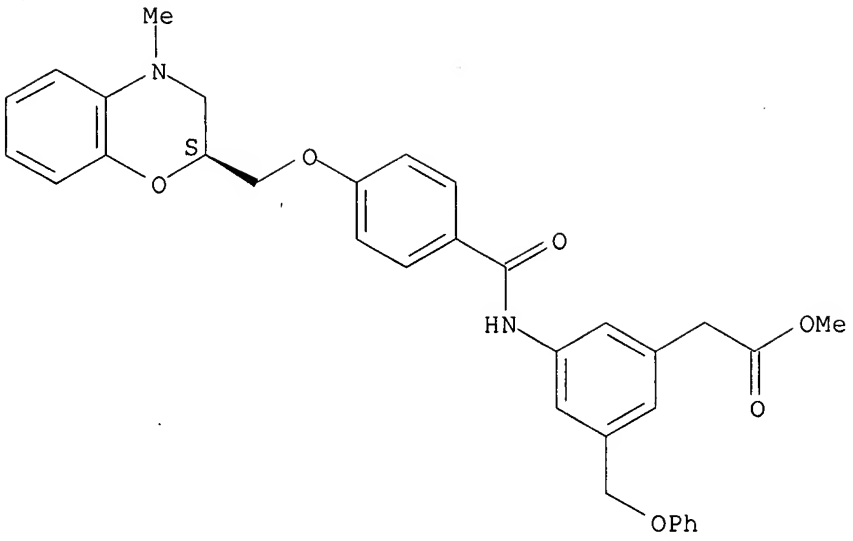
Absolute stereochemistry.



RN 603107-33-1 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-5-(phenoxymethyl)-, methyl ester (9CI) (CA INDEX NAME)

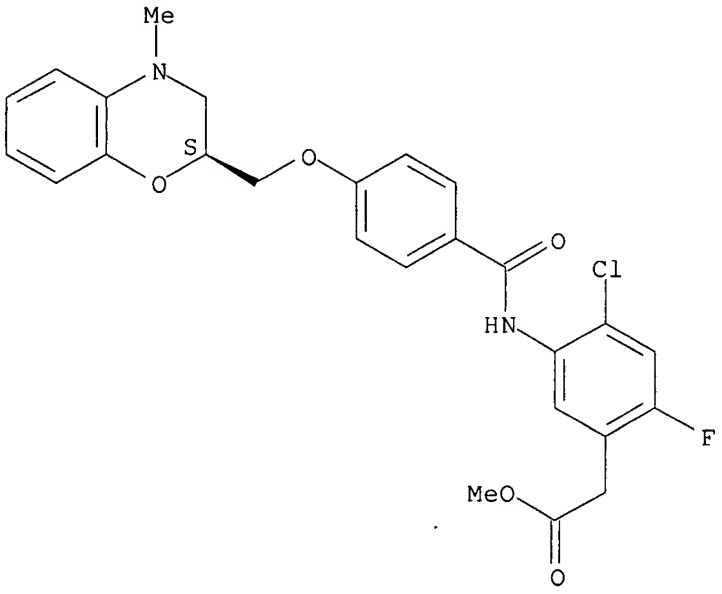
Absolute stereochemistry.

Updated Search



RN 603107-34-2 HCAPLUS
CN Benzeneacetic acid, 4-chloro-5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

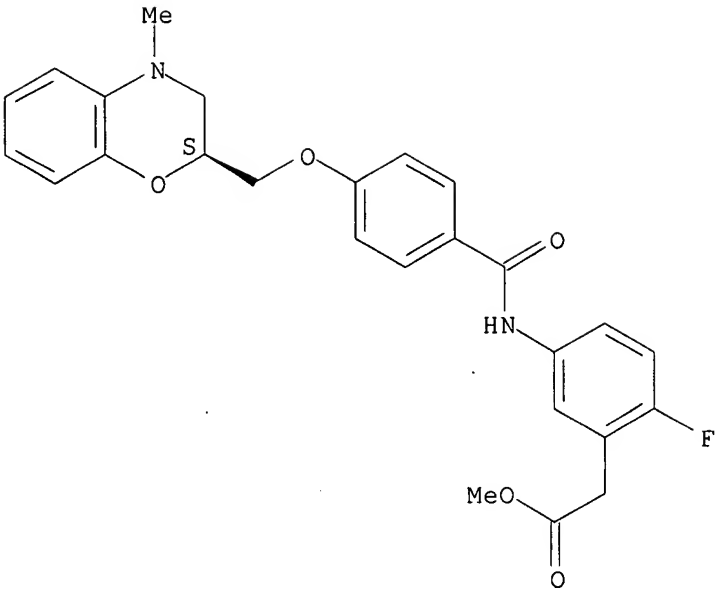
Absolute stereochemistry.



RN 603107-35-3 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

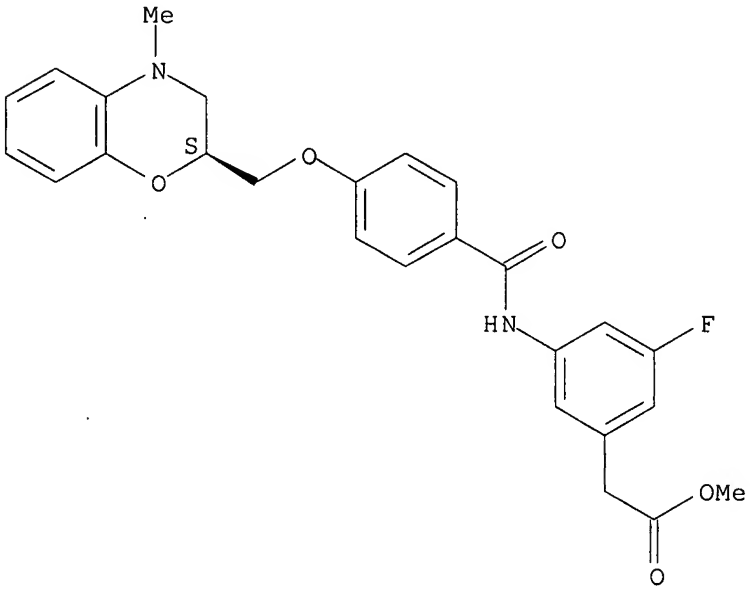
Absolute stereochemistry.

Updated Search



RN 603107-36-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-5-fluoro-, methyl ester (9CI) (CA INDEX NAME)

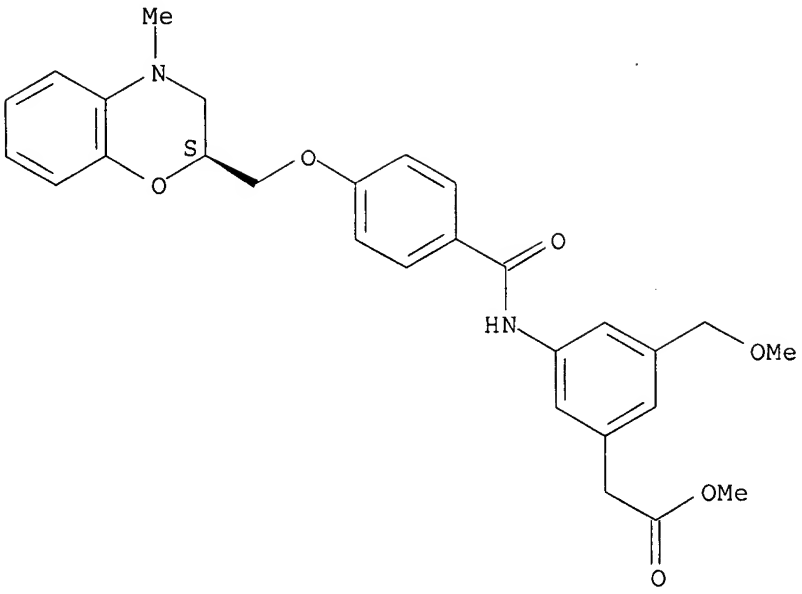
Absolute stereochemistry.



RN 603107-37-5 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-5-(methoxymethyl)-, methyl ester (9CI) (CA INDEX NAME)

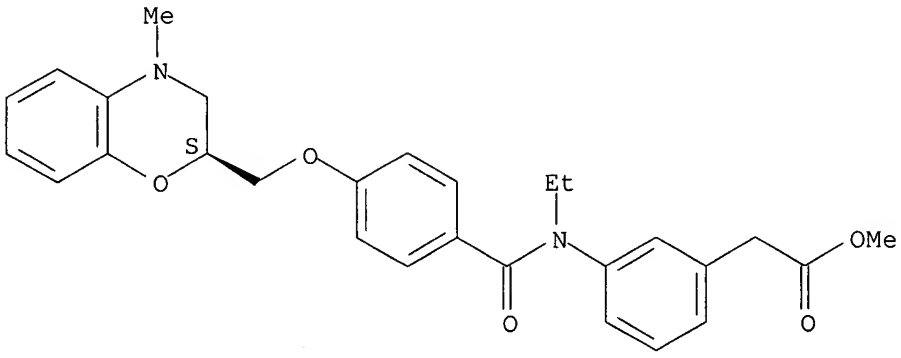
Absolute stereochemistry.

Updated Search



RN 603107-54-6 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]ethylamino]-, methyl ester (9CI) (CA INDEX NAME)

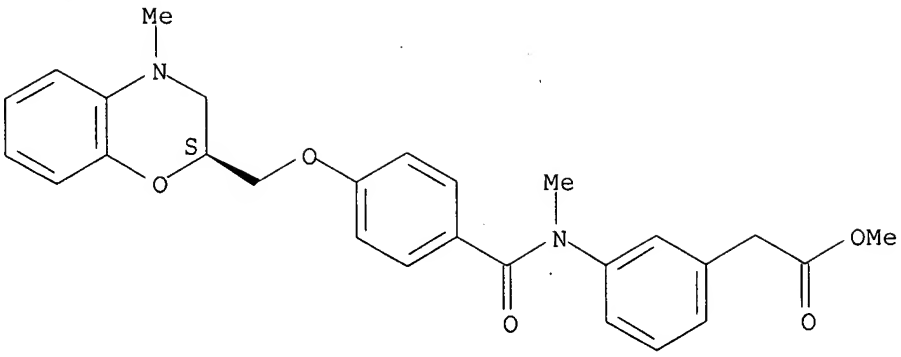
Absolute stereochemistry.



RN 603107-55-7 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]methylamino]-, methyl ester (9CI) (CA INDEX NAME)

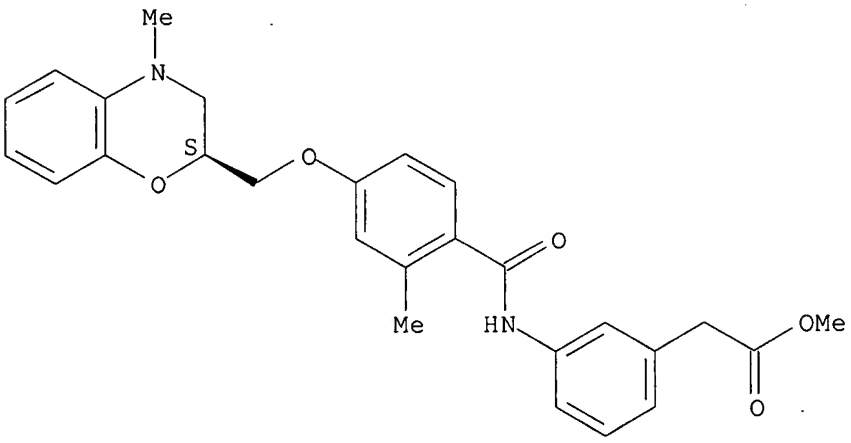
Absolute stereochemistry.

Updated Search



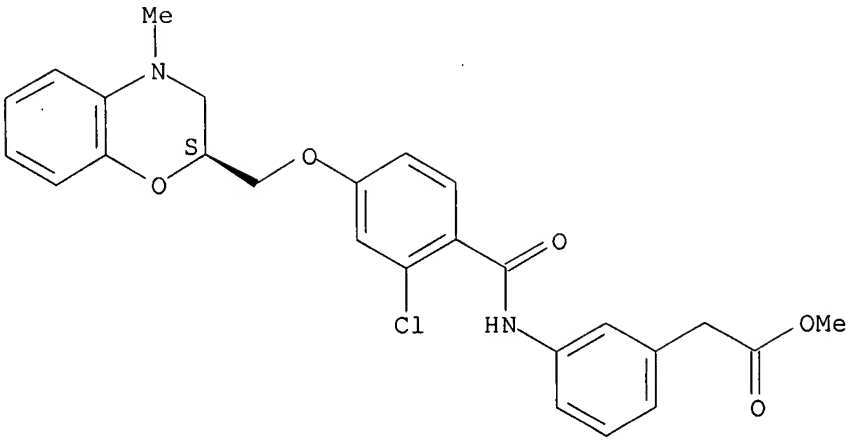
RN 603107-58-0 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



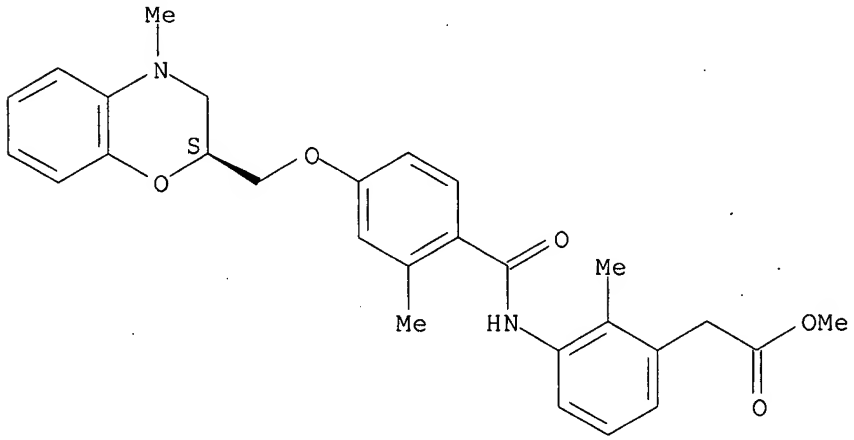
RN 603107-60-4 HCAPLUS
CN Benzeneacetic acid, 3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 603107-61-5 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)

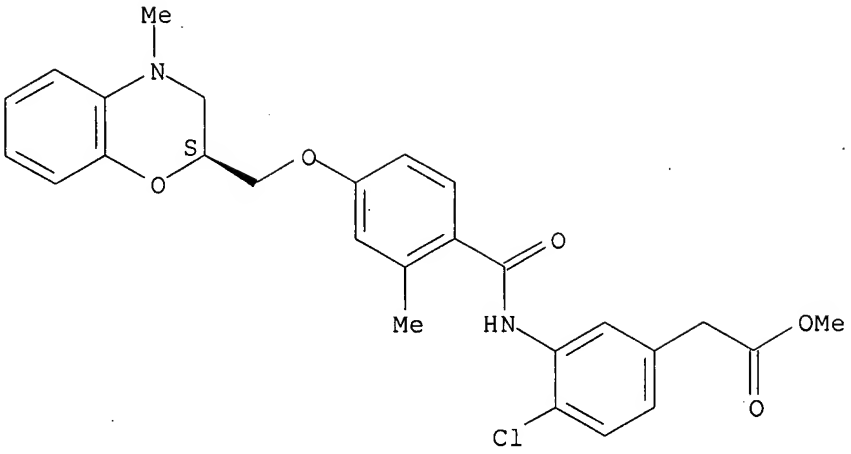
Absolute stereochemistry.



RN 603107-63-7 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

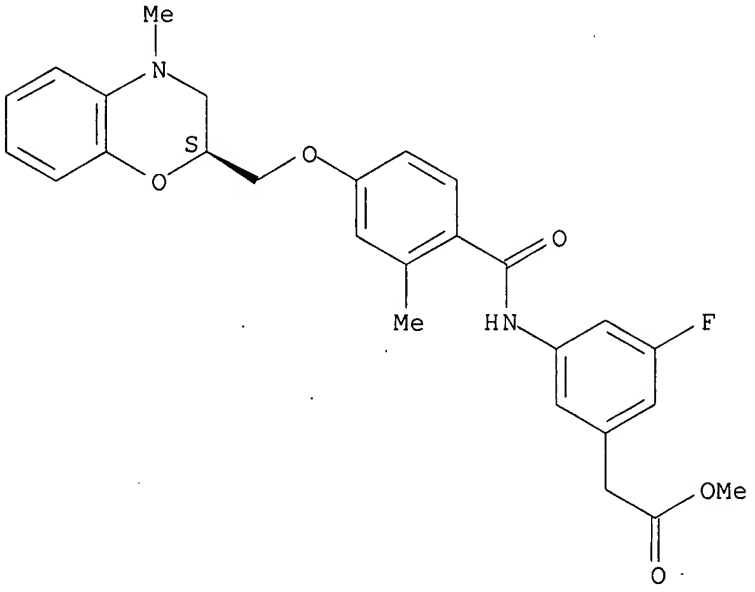
Absolute stereochemistry.

Updated Search



RN 603107-64-8 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-5-fluoro-, methyl ester (9CI) (CA INDEX NAME)

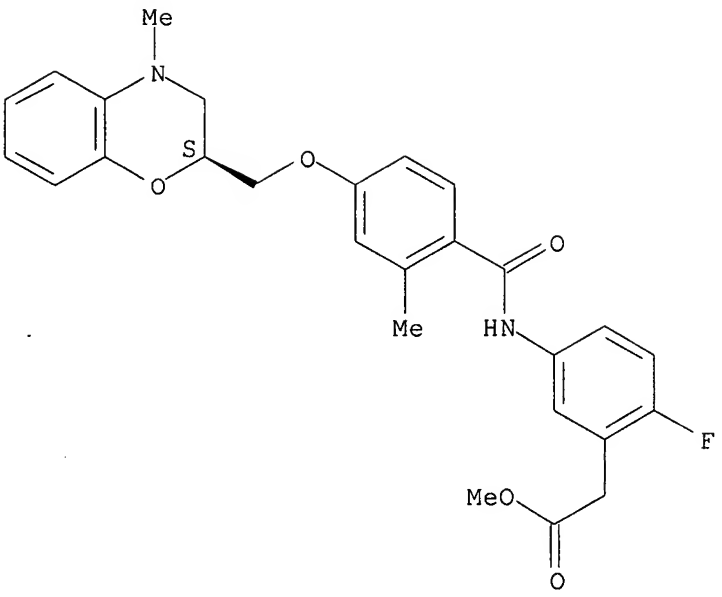
Absolute stereochemistry.



RN 603107-65-9 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

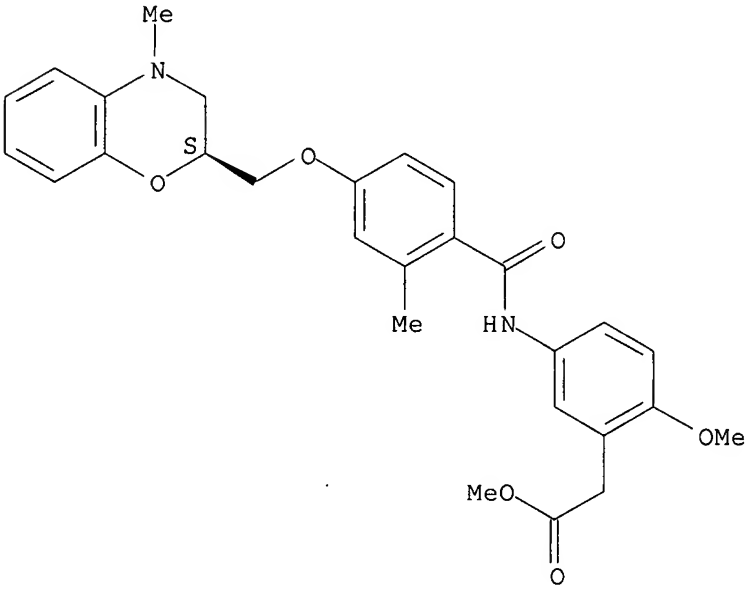
Absolute stereochemistry.

Updated Search



RN 603107-66-0 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-2-methoxy-, methyl ester (9CI) (CA INDEX NAME)

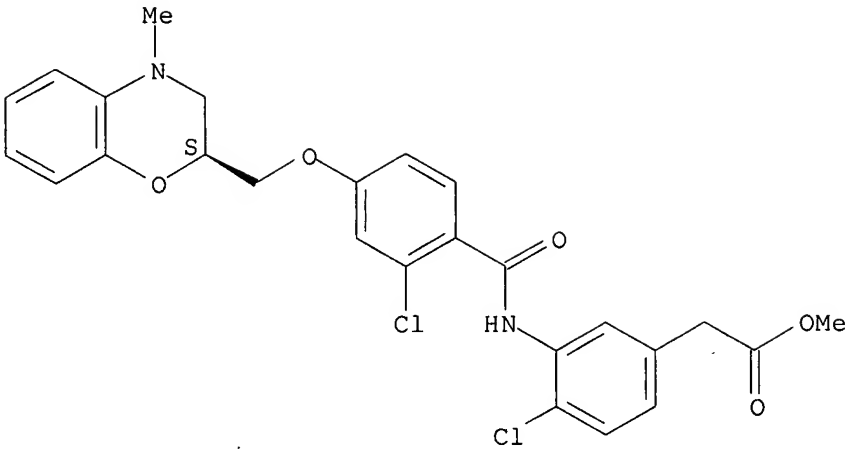
Absolute stereochemistry.



RN 603107-67-1 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

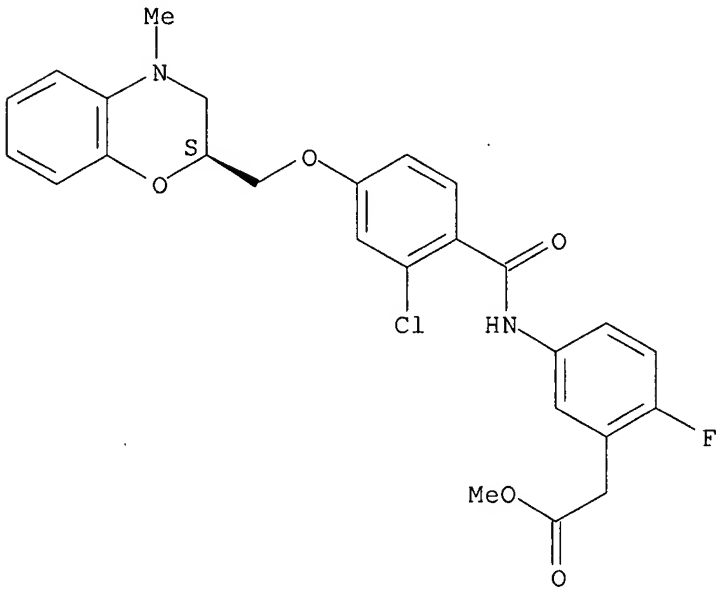
Absolute stereochemistry.

Updated Search



RN 603107-68-2 HCAPLUS
CN Benzeneacetic acid, 5-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

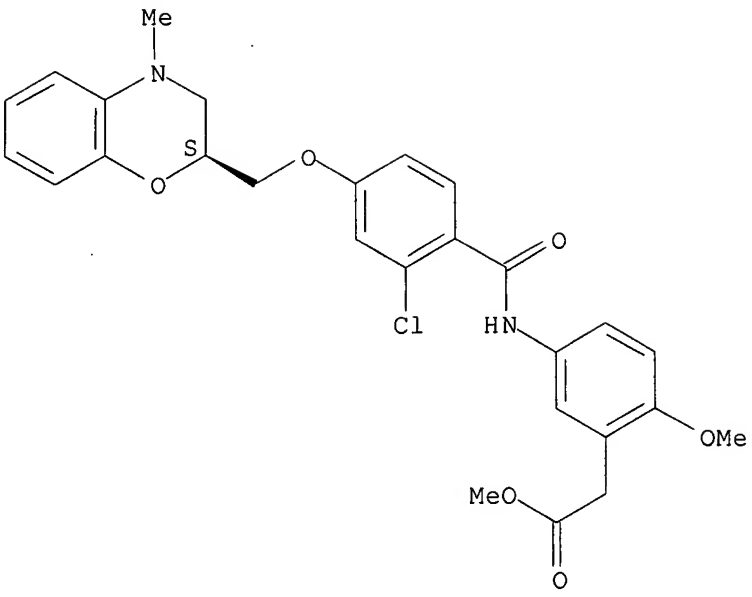
Absolute stereochemistry.



RN 603107-69-3 HCAPLUS
CN Benzeneacetic acid, 5-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methoxy-, methyl ester (9CI) (CA INDEX NAME)

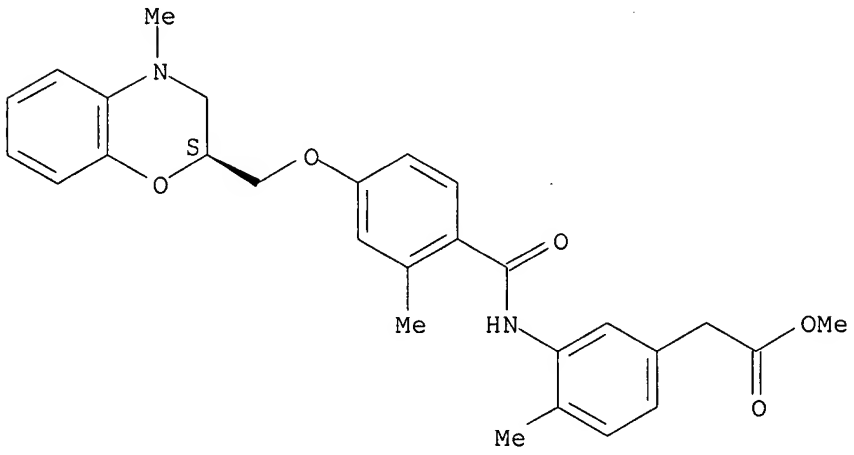
Absolute stereochemistry.

Updated Search



RN 603107-70-6 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-4-methyl-, methyl ester (9CI) (CA INDEX NAME)

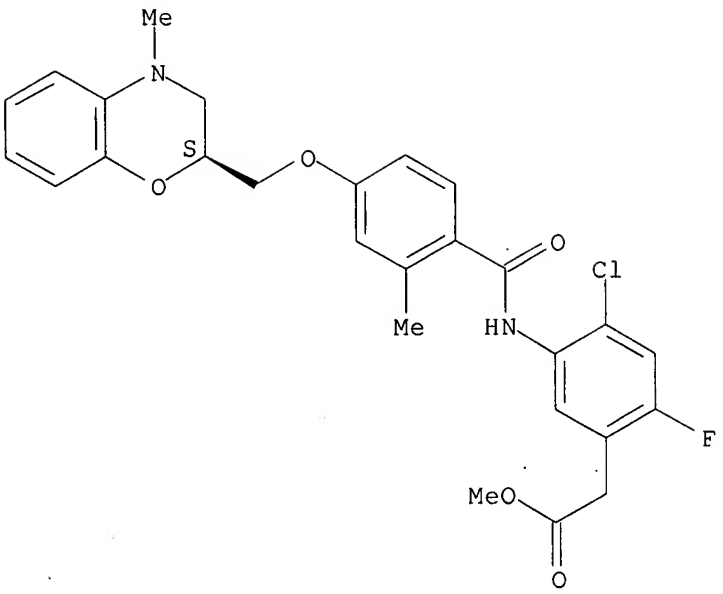
Absolute stereochemistry.



RN 603107-71-7 HCAPLUS
CN Benzeneacetic acid, 4-chloro-5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-2-fluoro-, methyl ester (9CI) (CA INDEX NAME)

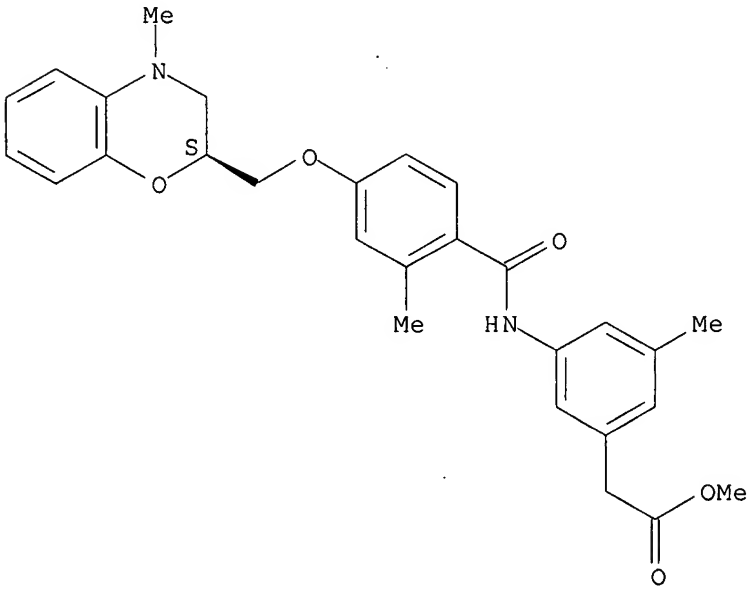
Absolute stereochemistry.

Updated Search



RN 603107-72-8 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-5-methyl-, methyl ester (9CI) (CA INDEX NAME)

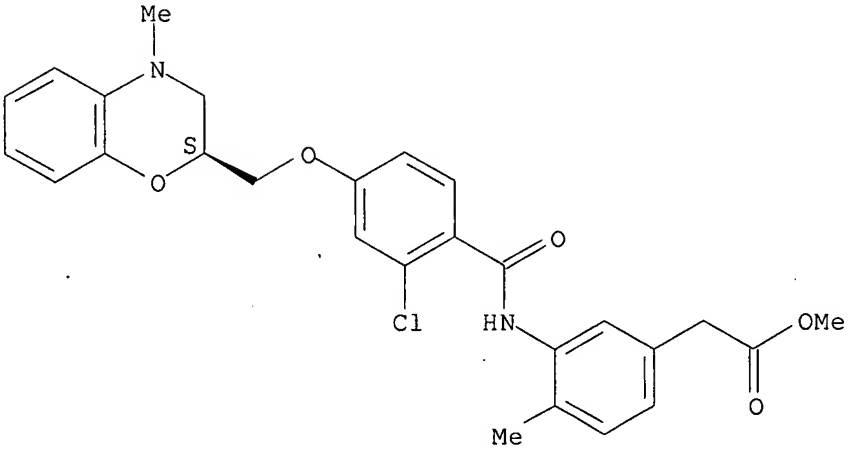
Absolute stereochemistry.



RN 603107-73-9 HCAPLUS
CN Benzeneacetic acid, 3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-methyl-, methyl ester (9CI) (CA INDEX NAME)

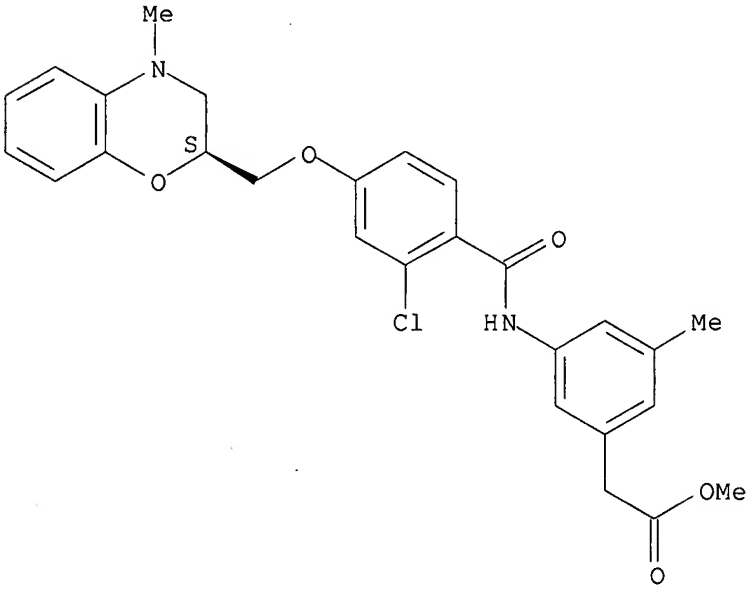
Absolute stereochemistry.

Updated Search



RN 603107-74-0 HCAPLUS
CN Benzeneacetic acid, 3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-5-methyl-, methyl ester (9CI) (CA INDEX NAME)

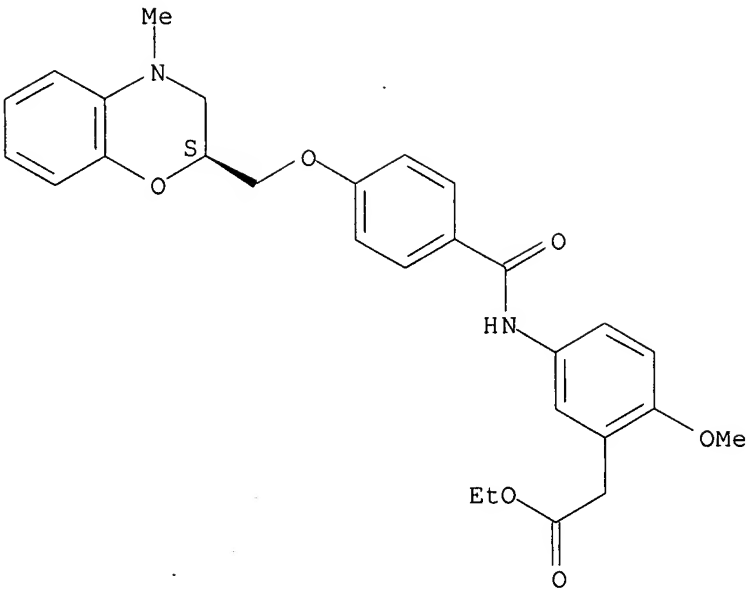
Absolute stereochemistry.



RN 603108-03-8 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

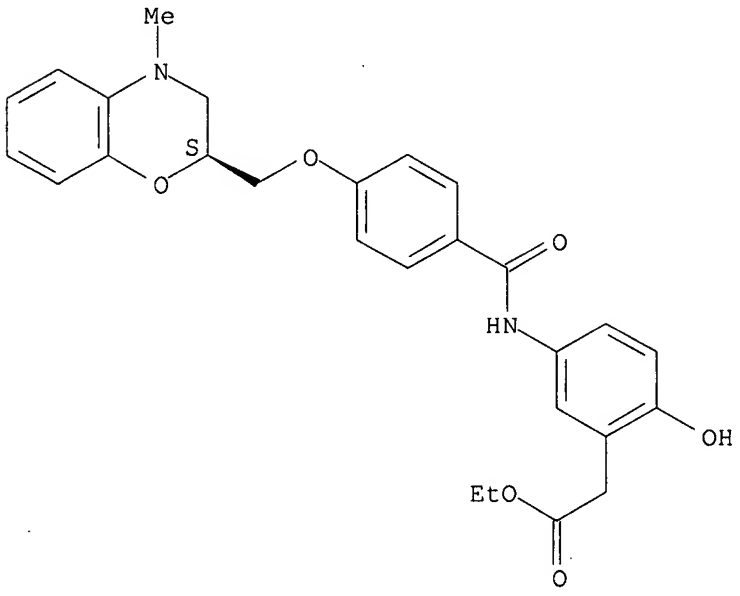
Absolute stereochemistry.

Updated Search



RN 603108-05-0 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)

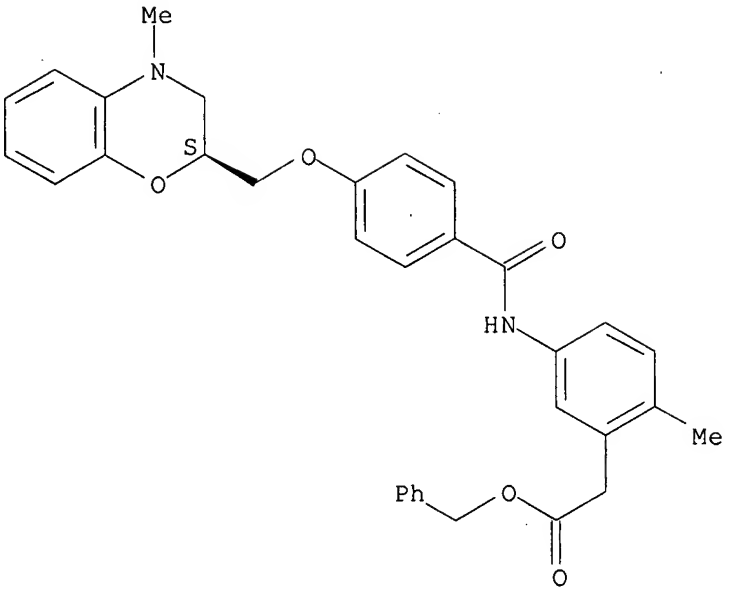
Absolute stereochemistry.



RN 603108-11-8 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

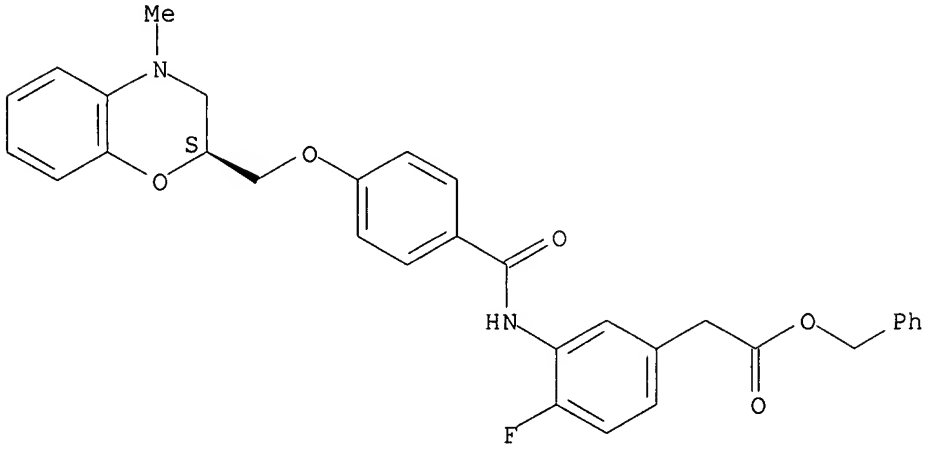
Absolute stereochemistry.

Updated Search



RN 603108-13-0 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-fluoro-, phenylmethyl ester (9CI) (CA INDEX NAME)

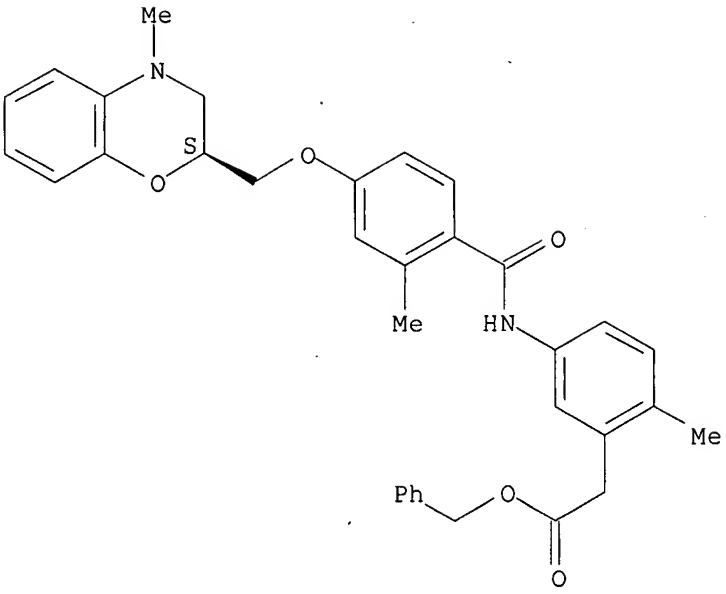
Absolute stereochemistry.



RN 603108-15-2 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-2-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

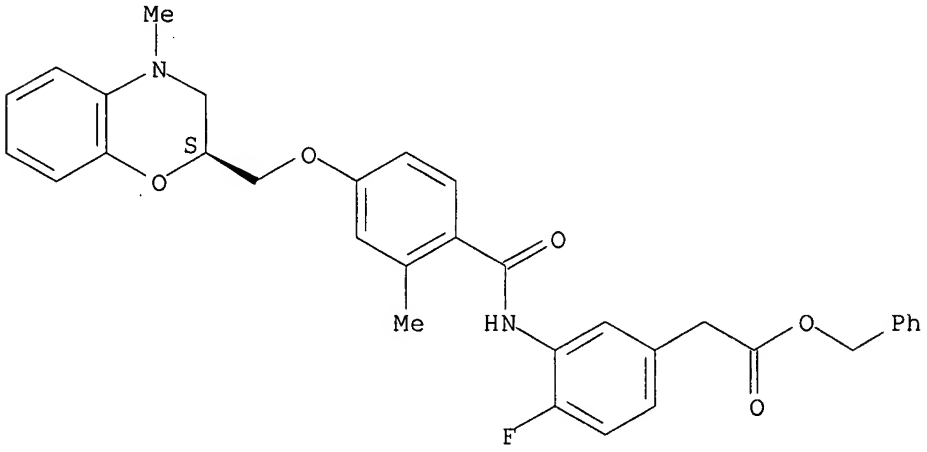
Absolute stereochemistry.

Updated Search



RN 603108-17-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-4-fluoro-, phenylmethyl ester (9CI) (CA INDEX NAME)

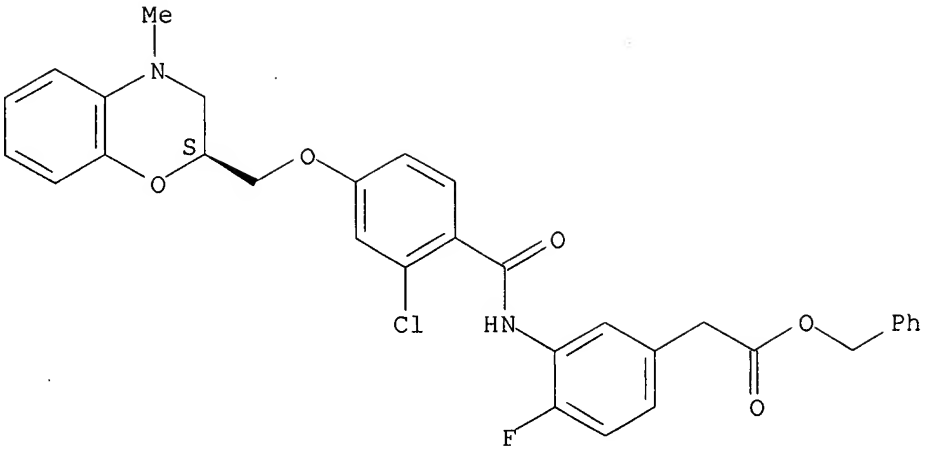
Absolute stereochemistry.



RN 603108-18-5 HCAPLUS
CN Benzeneacetic acid, 3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-fluoro-, phenylmethyl ester (9CI) (CA INDEX NAME)

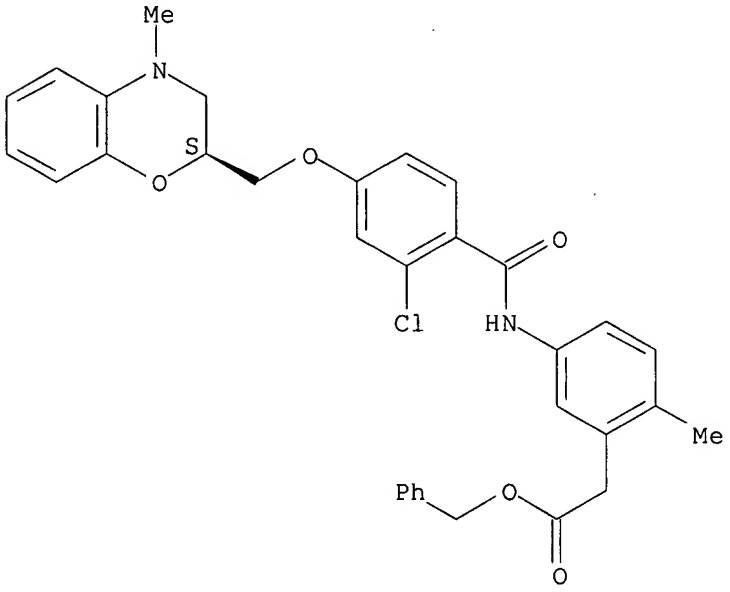
Absolute stereochemistry.

Updated Search



RN 603108-20-9 HCAPLUS
CN Benzeneacetic acid, 5-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

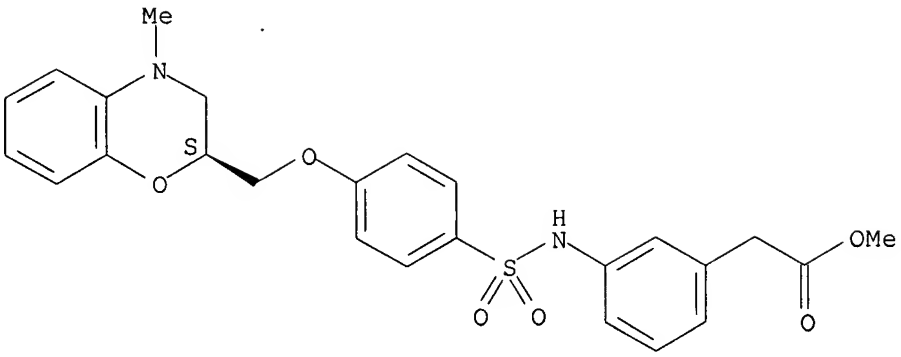
Absolute stereochemistry.



RN 603108-34-5 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]sulfonyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

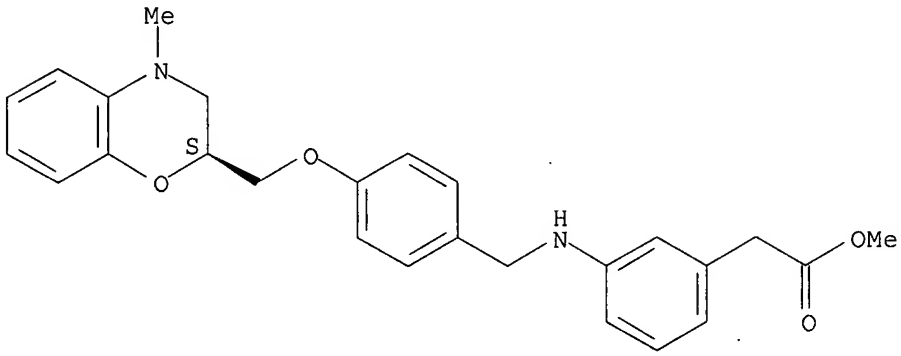
Absolute stereochemistry.

Updated Search



RN 603108-49-2 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 603107-38-6P 603107-39-7P 603107-40-0P
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603107-47-7P 603107-48-8P 603107-49-9P
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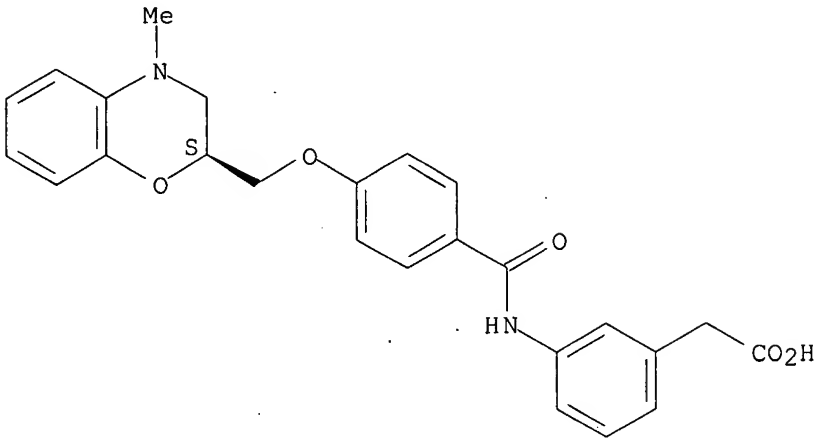
603108-43-6P 603108-45-8P 603108-47-0P
603108-51-6P 603108-53-8P 603108-55-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of aminophenylacetic acid derivs. as prostaglandin DP receptor antagonists)
RN 603107-38-6 HCAPLUS

Updated Search

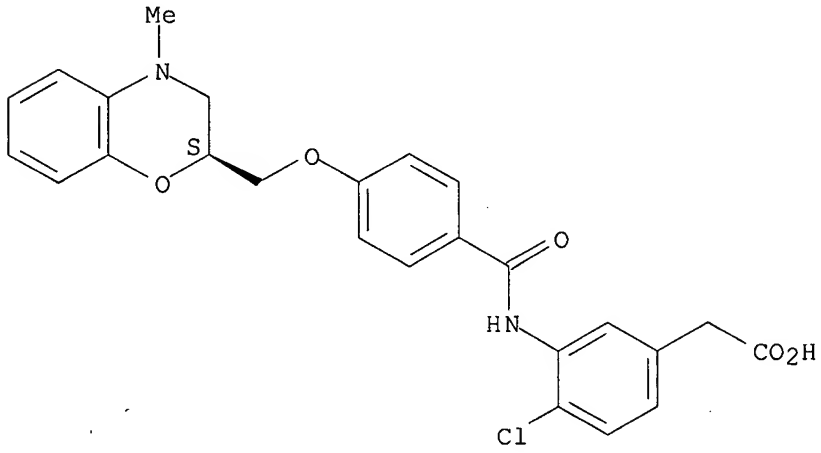
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 603107-39-7 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

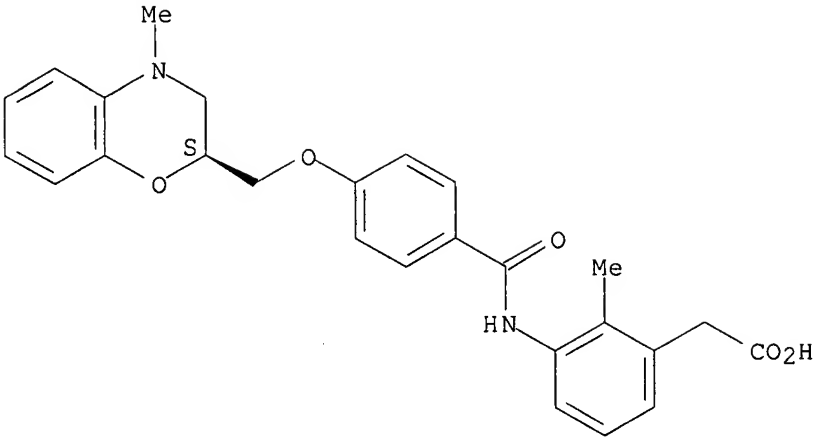
Absolute stereochemistry.



RN 603107-40-0 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

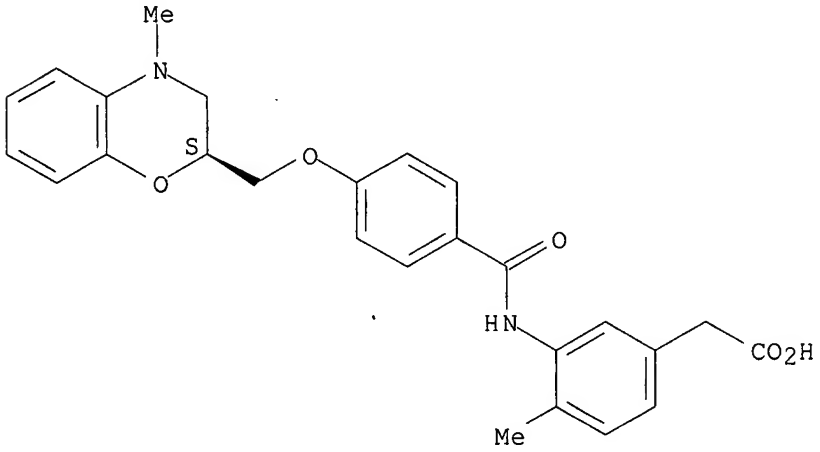
Absolute stereochemistry.

Updated Search



RN 603107-41-1 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

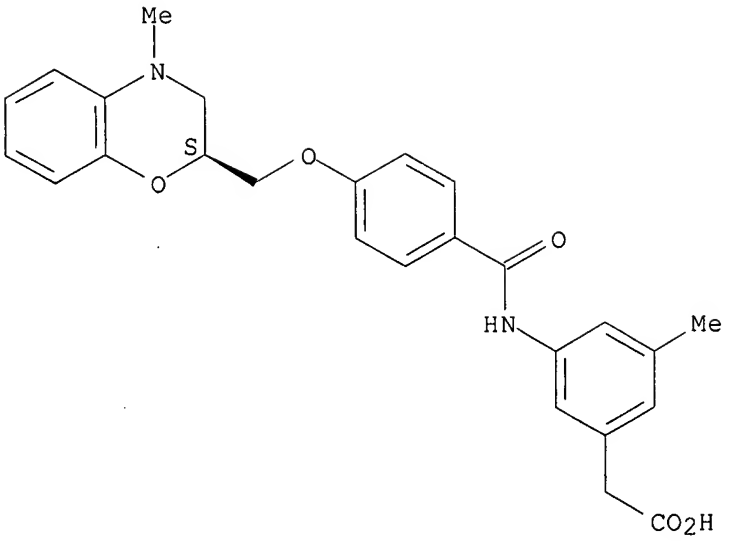
Absolute stereochemistry.



RN 603107-42-2 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-5-methyl- (9CI) (CA INDEX NAME)

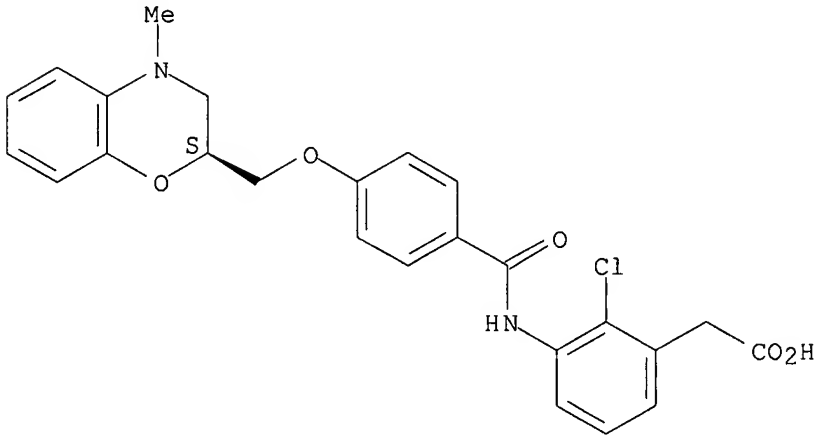
Absolute stereochemistry.

Updated Search



RN 603107-43-3 HCAPLUS
CN Benzeneacetic acid, 2-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

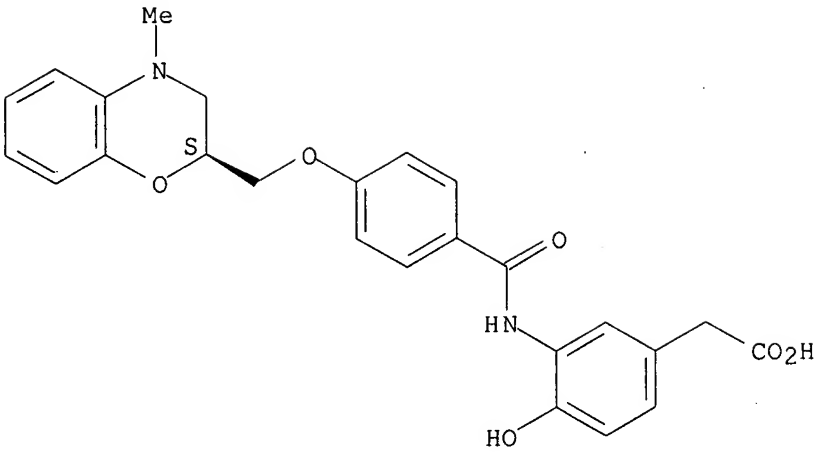
Absolute stereochemistry.



RN 603107-44-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-hydroxy- (9CI) (CA INDEX NAME)

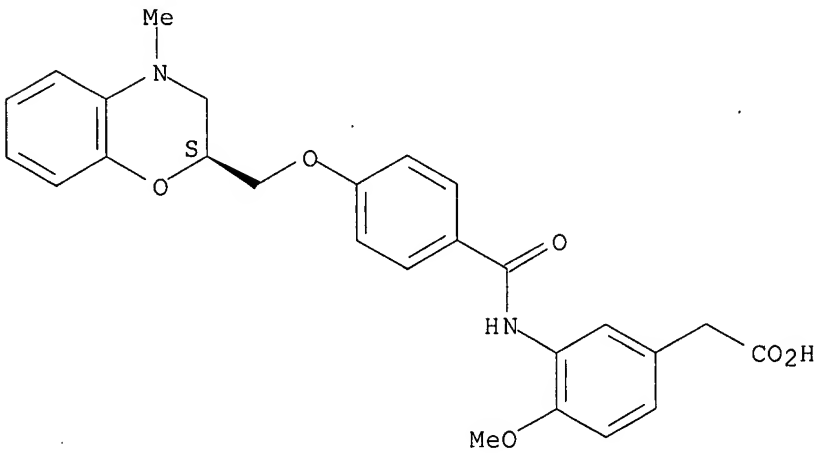
Absolute stereochemistry.

Updated Search



RN 603107-45-5 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-methoxy- (9CI) (CA INDEX NAME)

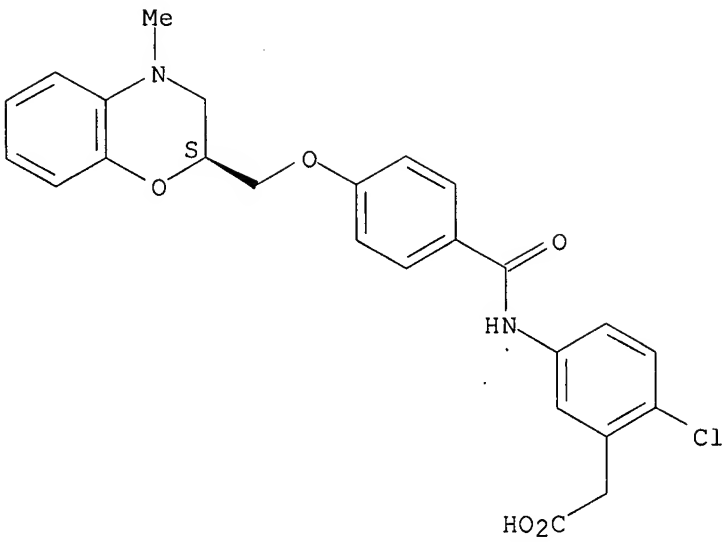
Absolute stereochemistry.



RN 603107-46-6 HCAPLUS
CN Benzeneacetic acid, 2-chloro-5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

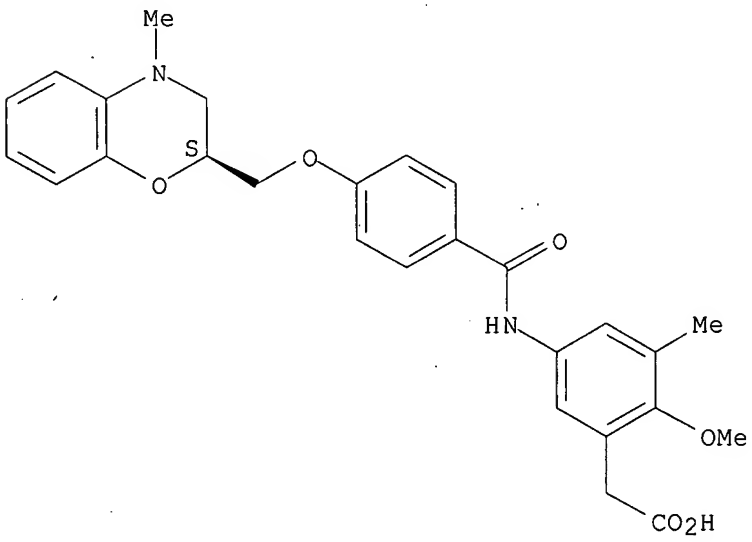
Absolute stereochemistry.

Updated Search



RN 603107-47-7 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methoxy-3-methyl- (9CI) (CA INDEX NAME)

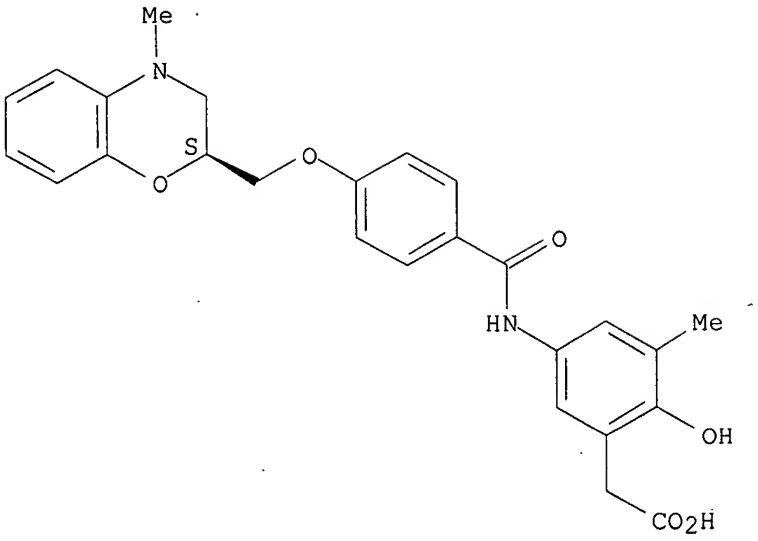
Absolute stereochemistry.



RN 603107-48-8 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-hydroxy-3-methyl- (9CI) (CA INDEX NAME)

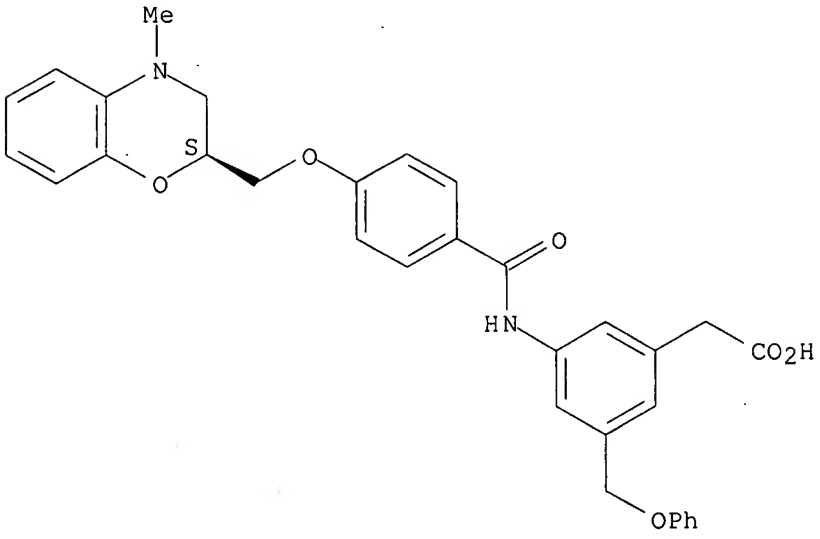
Absolute stereochemistry.

Updated Search



RN 603107-49-9 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-5-(phenoxymethyl)- (9CI) (CA INDEX NAME)

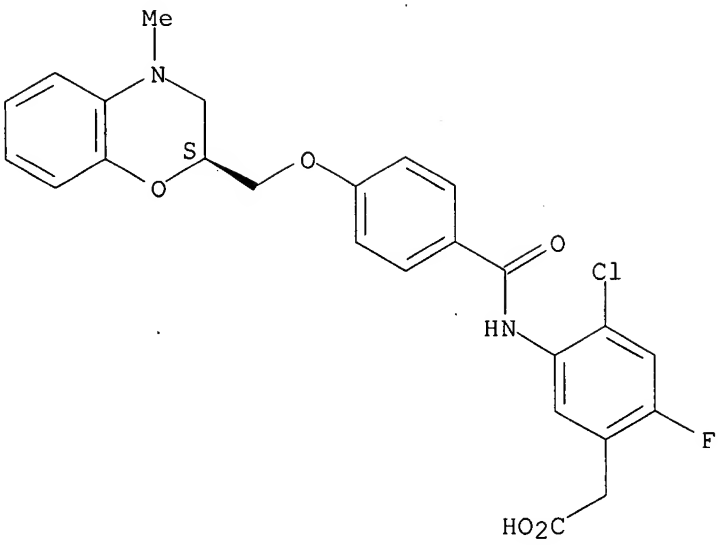
Absolute stereochemistry.



RN 603107-50-2 HCAPLUS
CN Benzeneacetic acid, 4-chloro-5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-fluoro- (9CI) (CA INDEX NAME)

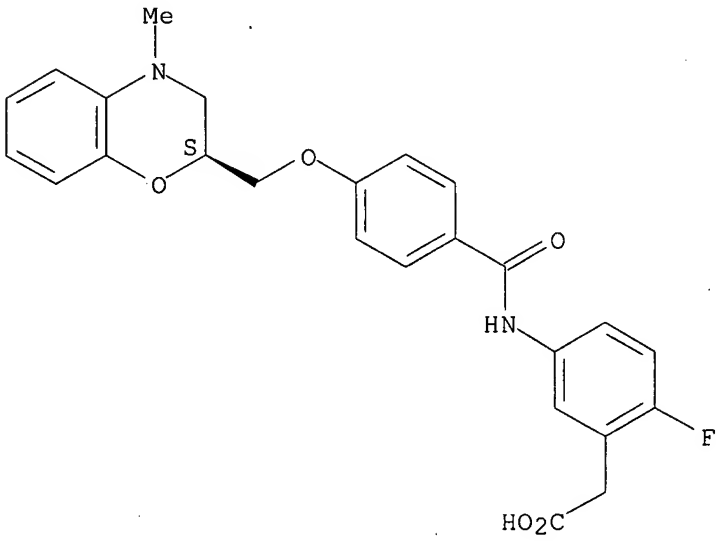
Absolute stereochemistry.

Updated Search



RN 603107-51-3 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-fluoro- (9CI) (CA INDEX NAME)

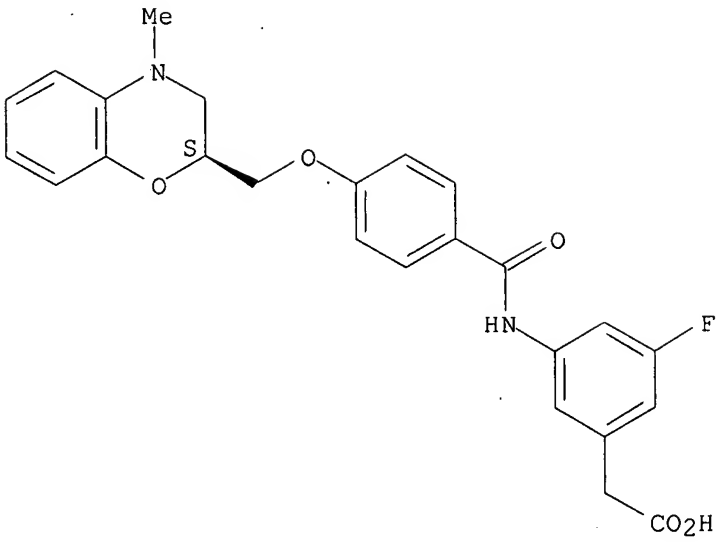
Absolute stereochemistry.



RN 603107-52-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-5-fluoro- (9CI) (CA INDEX NAME)

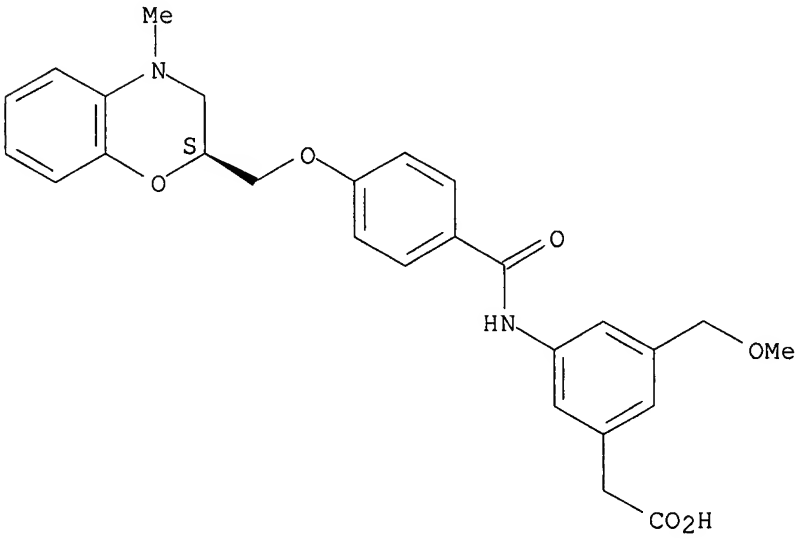
Absolute stereochemistry.

Updated Search



RN 603107-53-5 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-5-(methoxymethyl)- (9CI) (CA INDEX NAME)

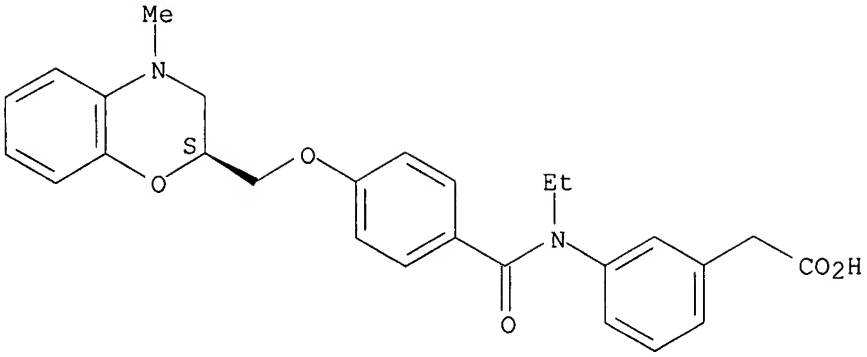
Absolute stereochemistry.



RN 603107-56-8 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]ethylamino]- (9CI) (CA INDEX NAME)

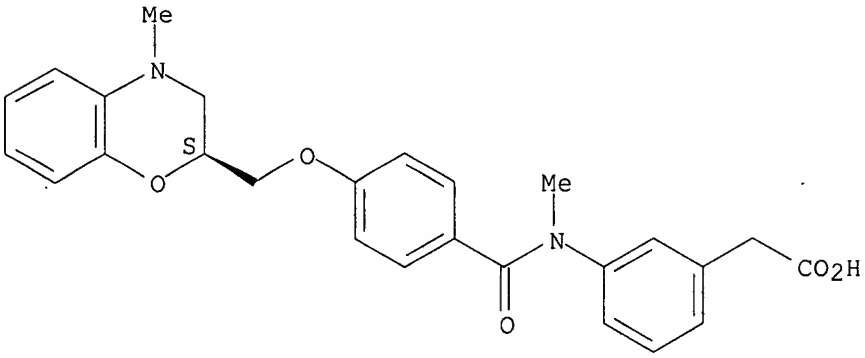
Absolute stereochemistry.

Updated Search



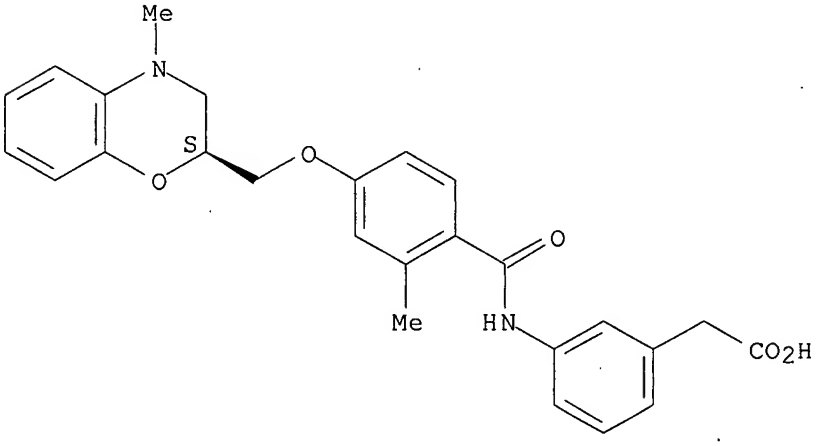
RN 603107-57-9 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 603107-75-1 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]- (9CI) (CA INDEX NAME)

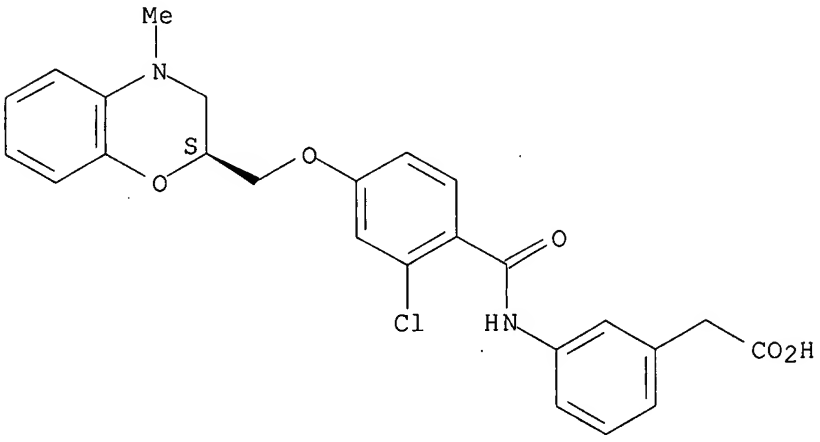
Absolute stereochemistry.



Updated Search

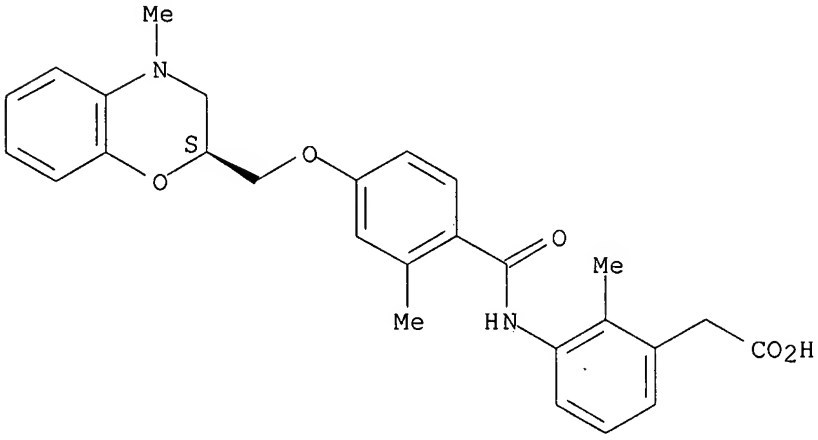
RN 603107-77-3 HCAPLUS
CN Benzeneacetic acid, 3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 603107-79-5 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

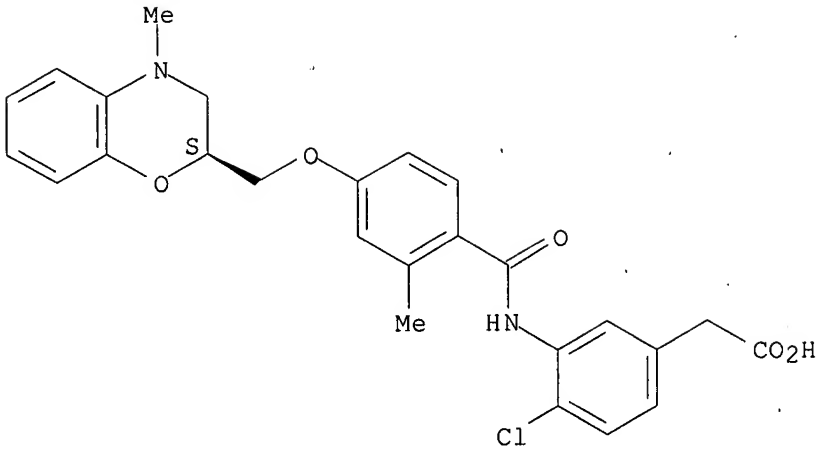
Absolute stereochemistry.



RN 603107-80-8 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]- (9CI) (CA INDEX NAME)

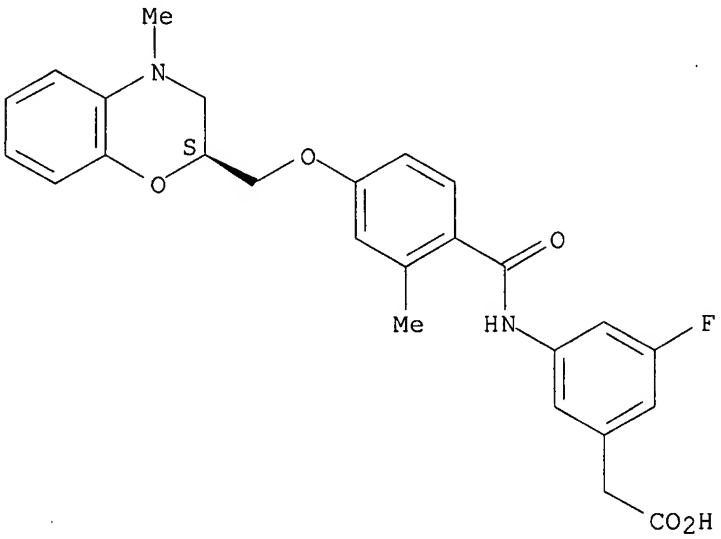
Absolute stereochemistry.

Updated Search



RN 603107-82-0 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-5-fluoro- (9CI) (CA INDEX NAME)

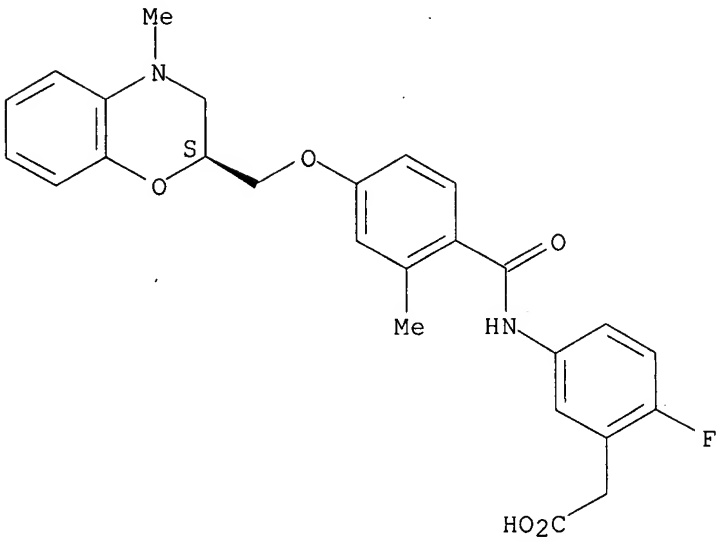
Absolute stereochemistry.



RN 603107-84-2 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-2-fluoro- (9CI) (CA INDEX NAME)

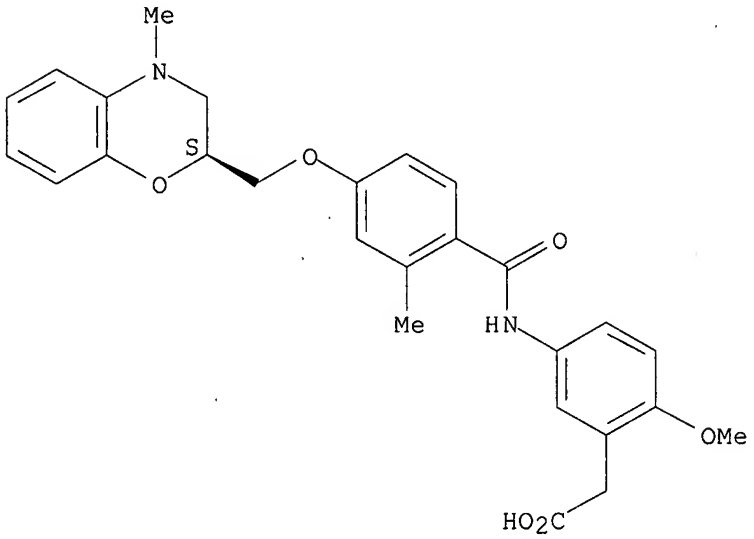
Absolute stereochemistry.

Updated Search



RN 603107-86-4 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-2-methoxy- (9CI) (CA INDEX NAME)

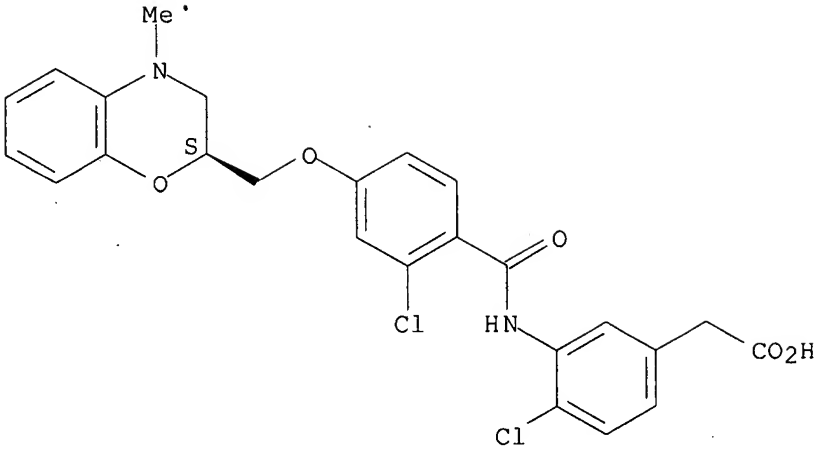
Absolute stereochemistry.



RN 603107-88-6 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

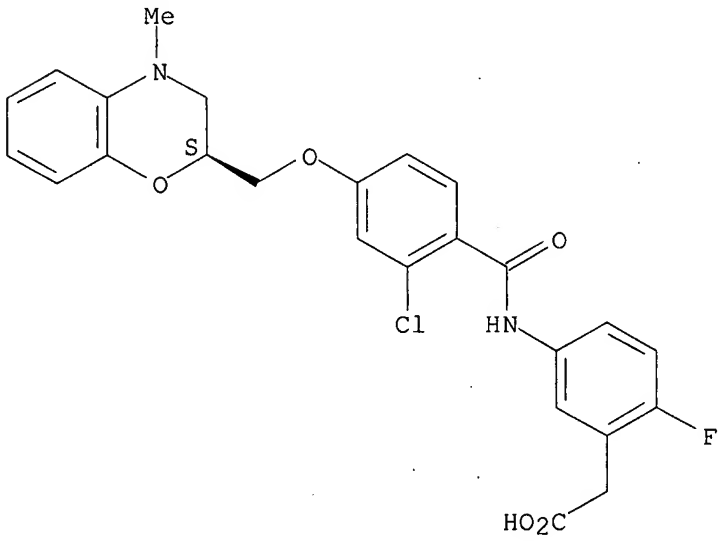
Absolute stereochemistry.

Updated Search



RN 603107-90-0 HCAPLUS
CN Benzeneacetic acid, 5-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-fluoro- (9CI) (CA INDEX NAME)

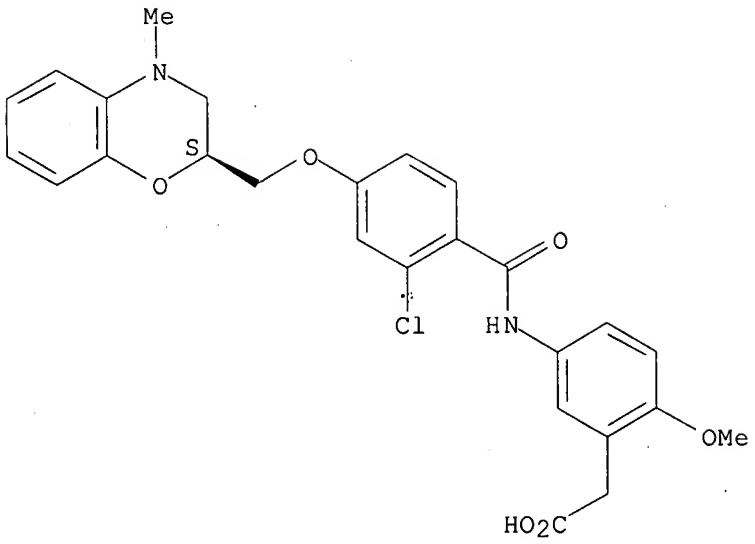
Absolute stereochemistry.



RN 603107-92-2 HCAPLUS
CN Benzeneacetic acid, 5-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methoxy- (9CI) (CA INDEX NAME)

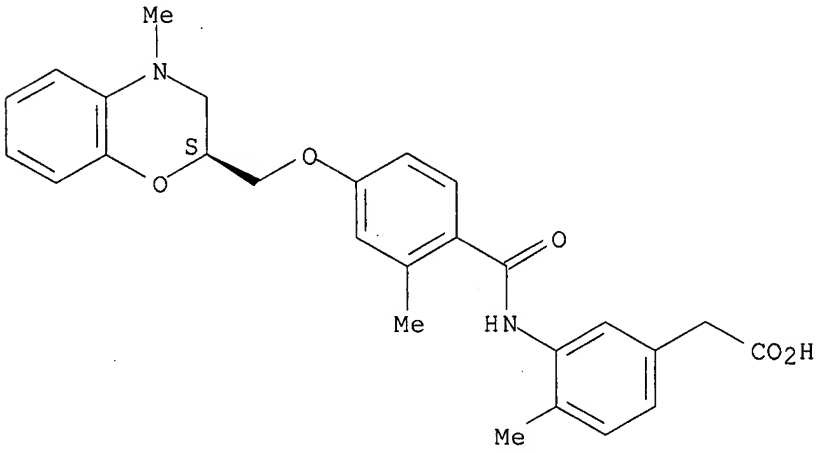
Absolute stereochemistry.

Updated Search



RN 603107-94-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

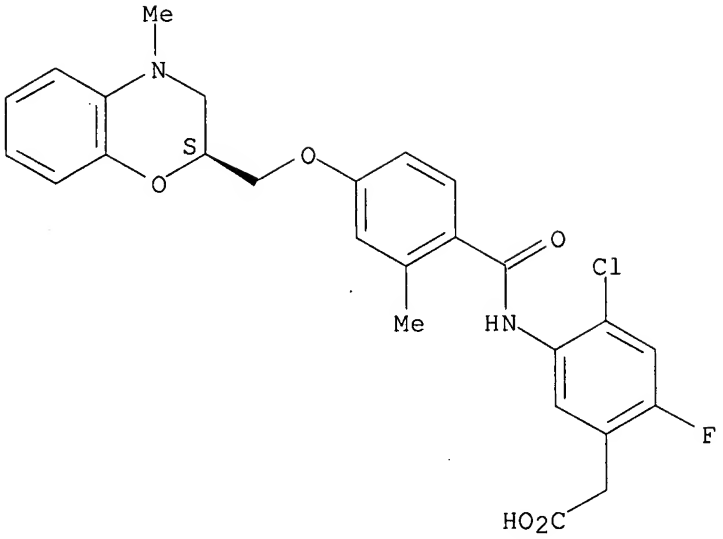
Absolute stereochemistry.



RN 603107-96-6 HCAPLUS
CN Benzeneacetic acid, 4-chloro-5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-2-fluoro- (9CI) (CA INDEX NAME)

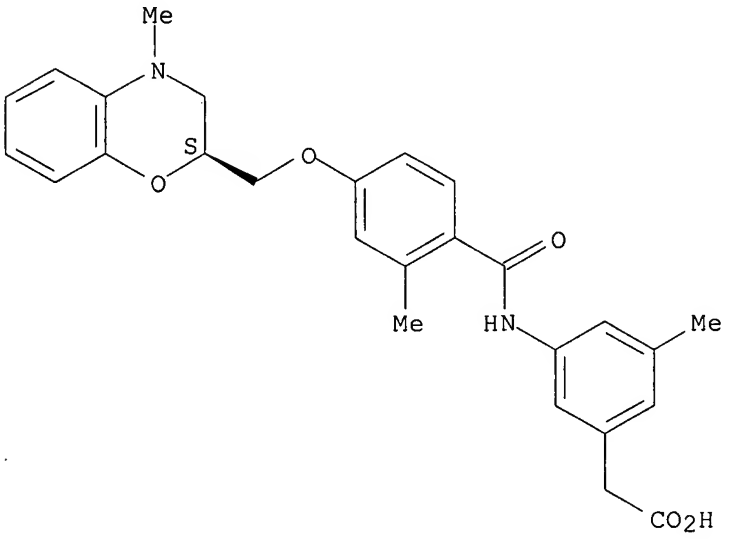
Absolute stereochemistry.

Updated Search



RN 603107-98-8 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 603107-99-9 HCAPLUS
CN Benzeneacetic acid, 3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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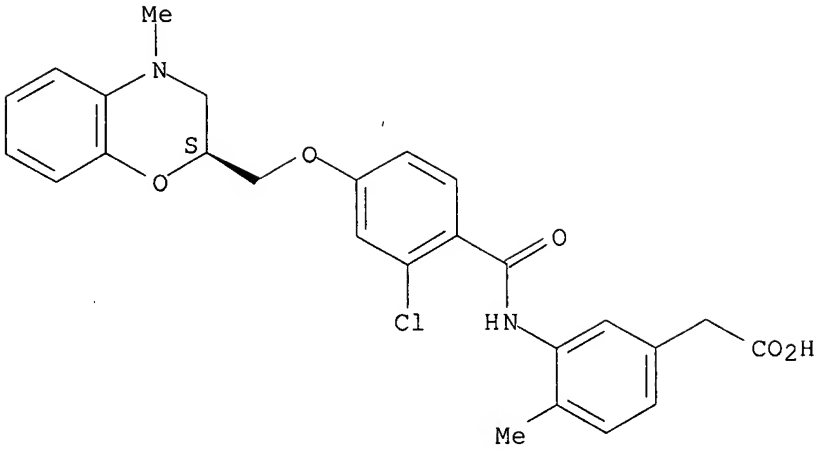

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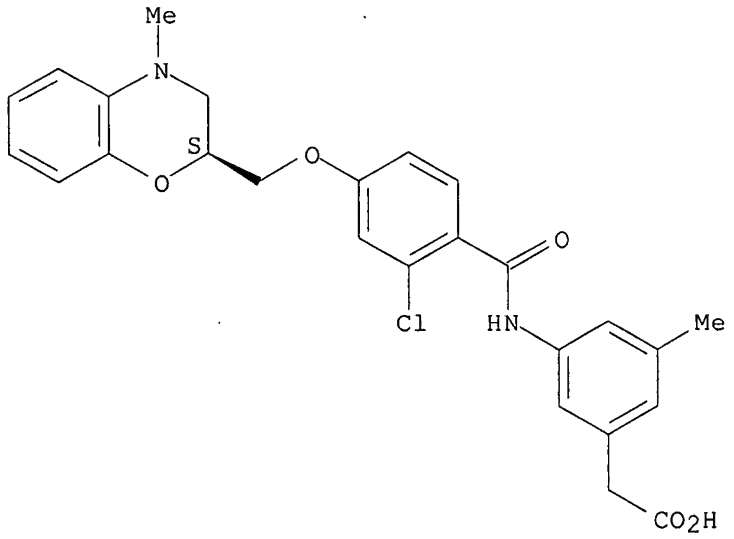
CN Benzeneacetic acid, 3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-5-methyl- (9CI) (CA INDEX NAME)

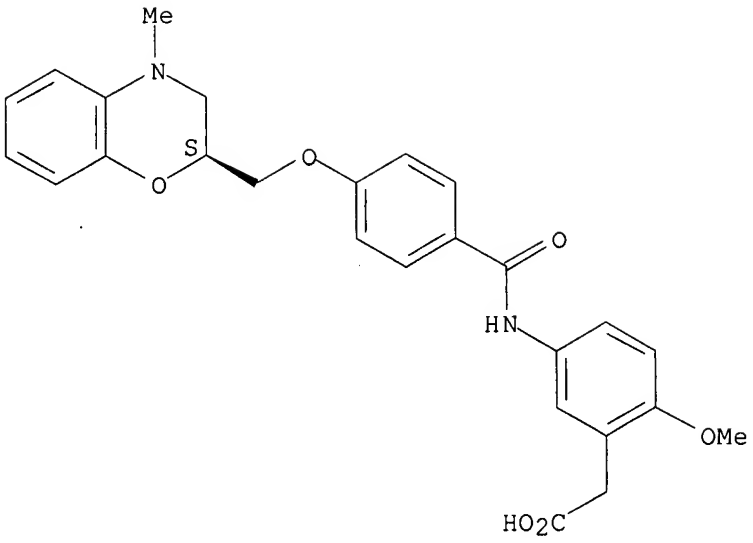
Absolute stereochemistry.



RN 603108-07-2 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Updated Search



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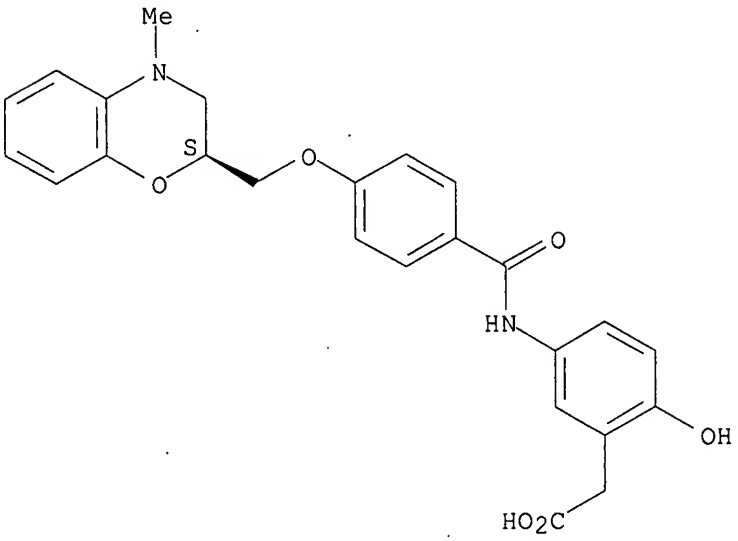
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-hydroxy- (9CI) (CA INDEX NAME)

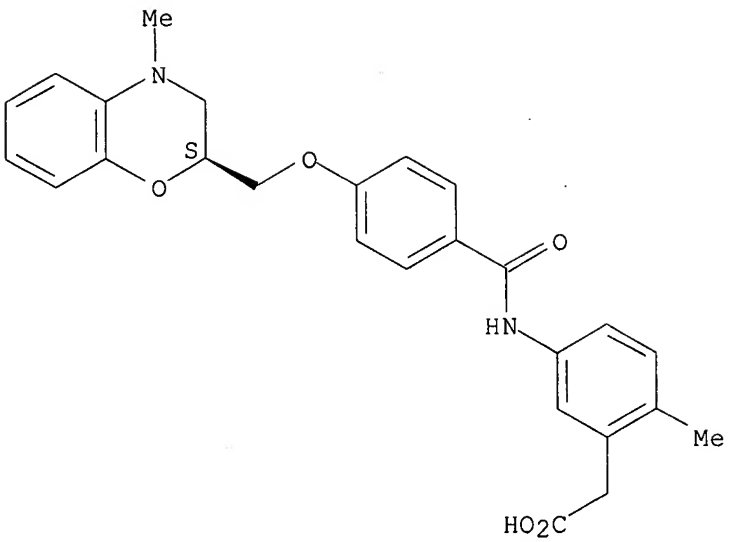
Absolute stereochemistry.



RN 603108-22-1 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

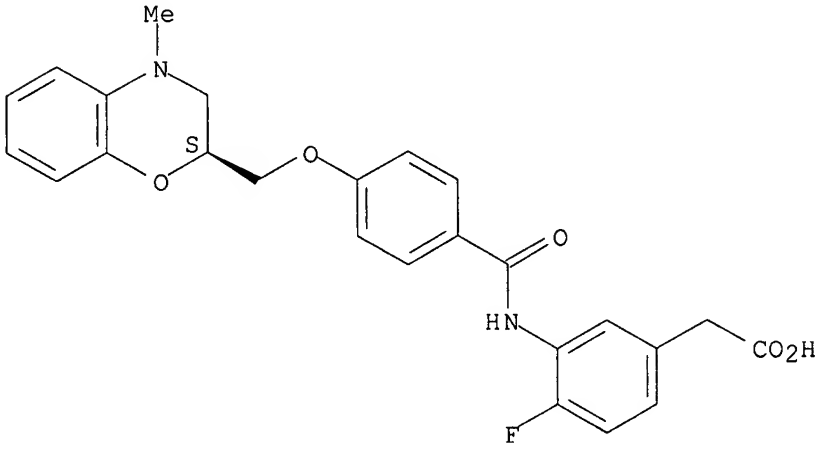
Absolute stereochemistry.

Updated Search



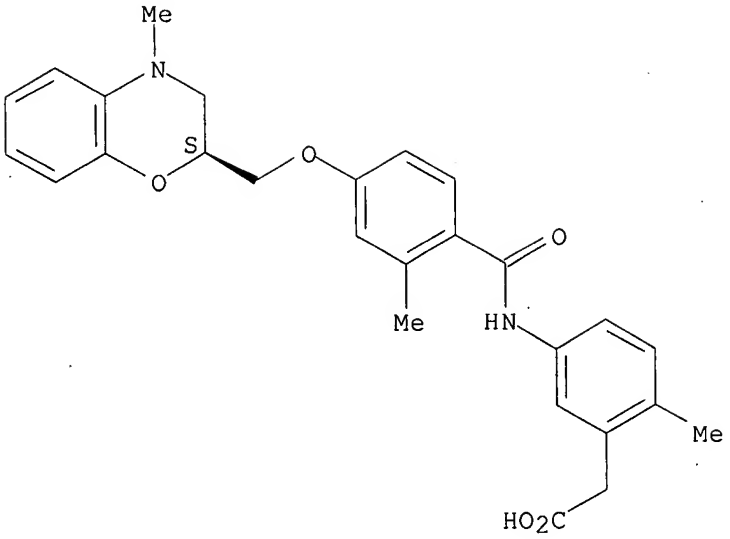
RN 603108-24-3 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



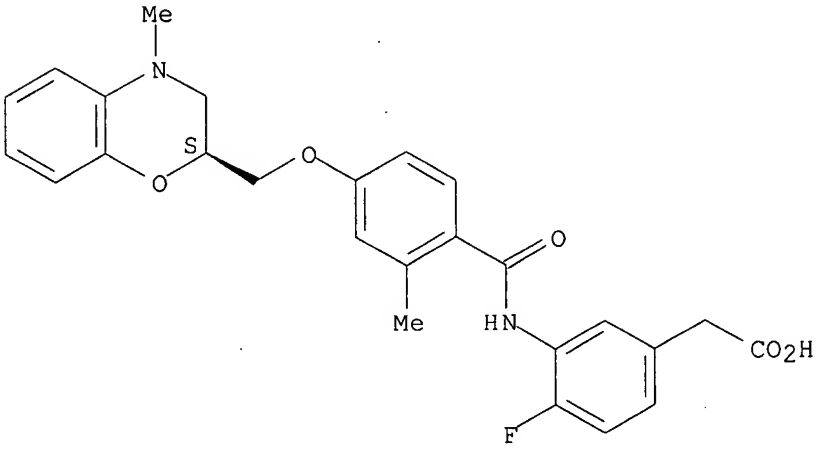
RN 603108-26-5 HCAPLUS
CN Benzeneacetic acid, 5-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 603108-28-7 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2-methylbenzoyl]amino]-4-fluoro- (9CI) (CA INDEX NAME)

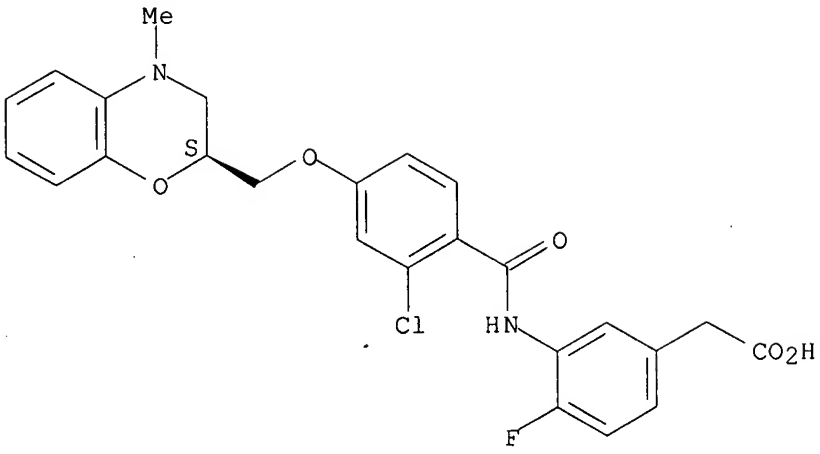
Absolute stereochemistry.



RN 603108-30-1 HCAPLUS
CN Benzeneacetic acid, 3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-4-fluoro- (9CI) (CA INDEX NAME)

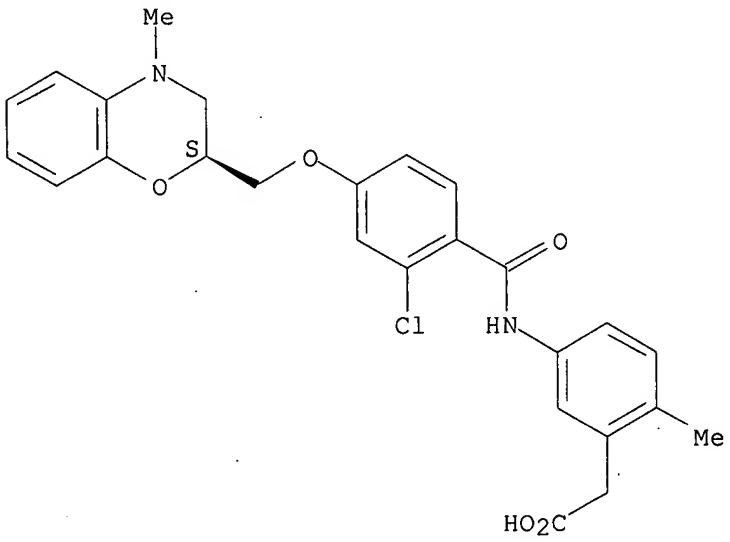
Absolute stereochemistry.

Updated Search



RN 603108-32-3 HCAPLUS
CN Benzeneacetic acid, 5-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-2-methyl- (9CI) (CA INDEX NAME)

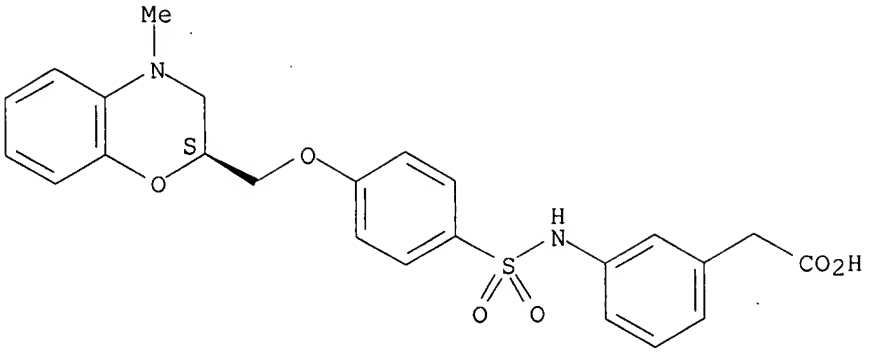
Absolute stereochemistry.



RN 603108-36-7 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]sulfonyl]amino]- (9CI) (CA INDEX NAME)

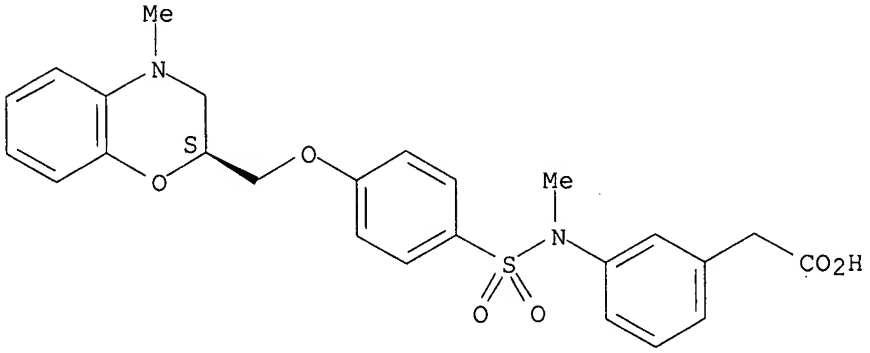
Absolute stereochemistry.

Updated Search



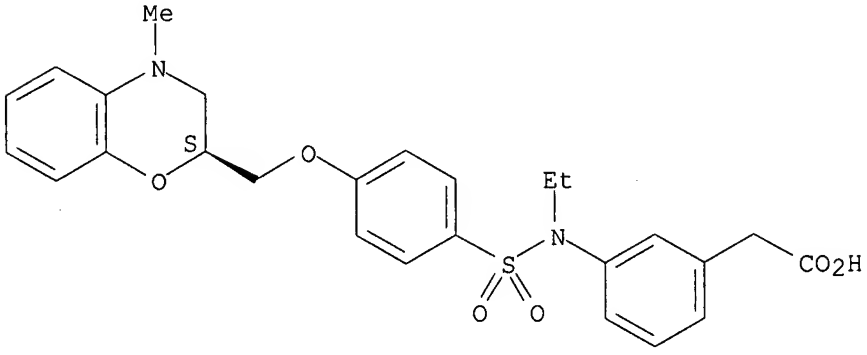
RN 603108-38-9 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]sulfonyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 603108-39-0 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]sulfonyl]ethylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

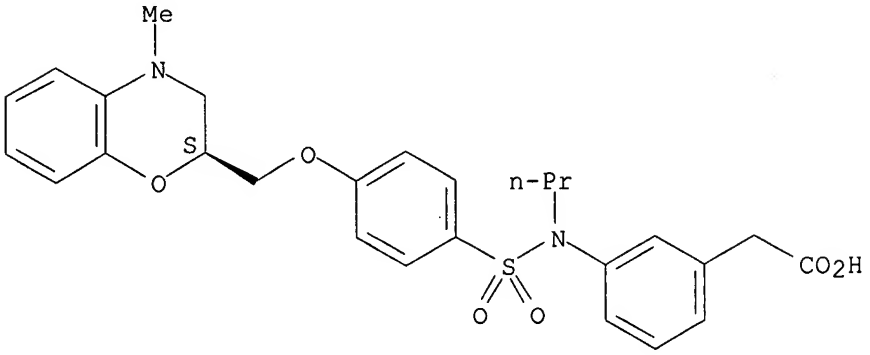


RN 603108-41-4 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-

Updated Search

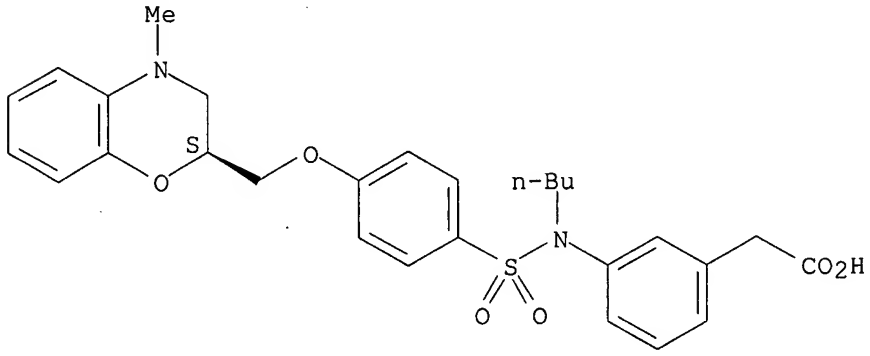
yl]methoxy]phenyl]sulfonyl]propylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



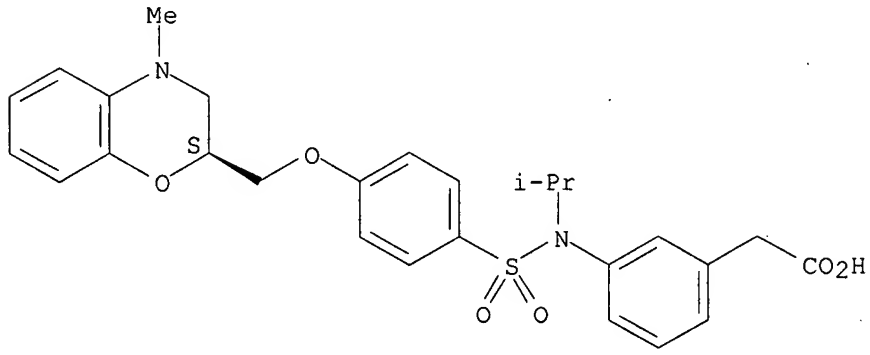
RN 603108-43-6 HCAPLUS
CN Benzeneacetic acid, 3-[butyl[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]sulfonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 603108-45-8 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]sulfonyl](1-methylethyl)amino]- (9CI) (CA INDEX NAME)

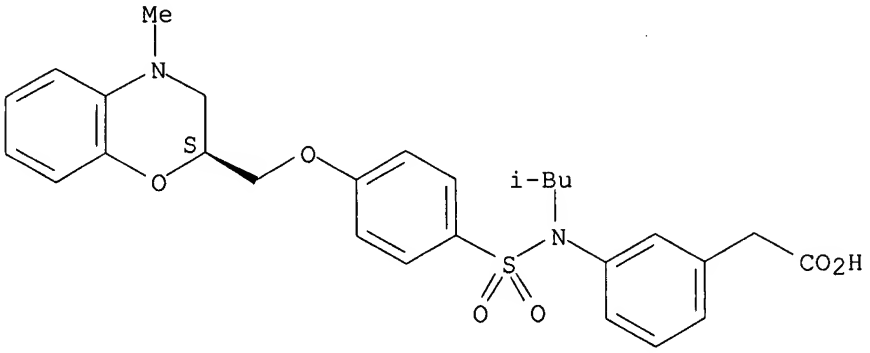
Absolute stereochemistry.



Updated Search

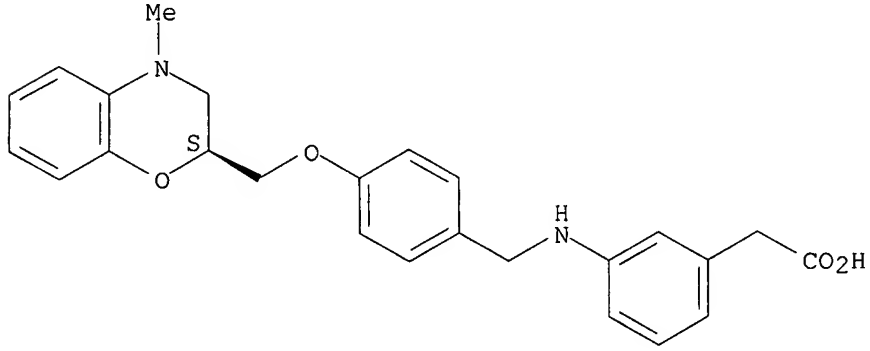
RN 603108-47-0 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]sulfonyl](2-methylpropyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 603108-51-6 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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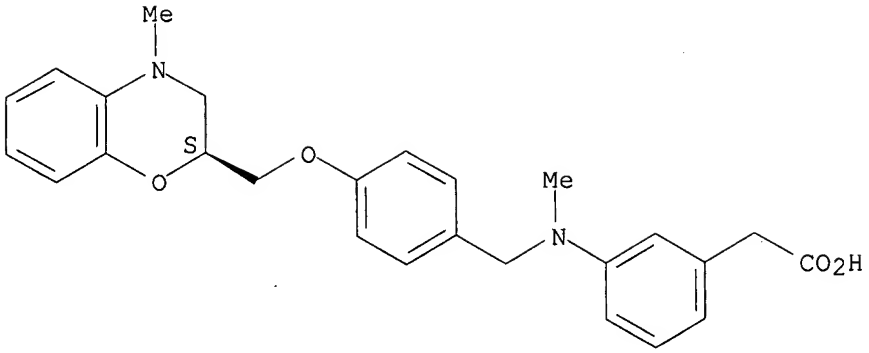
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]methyl]methylamino]- (9CI) (CA INDEX NAME)

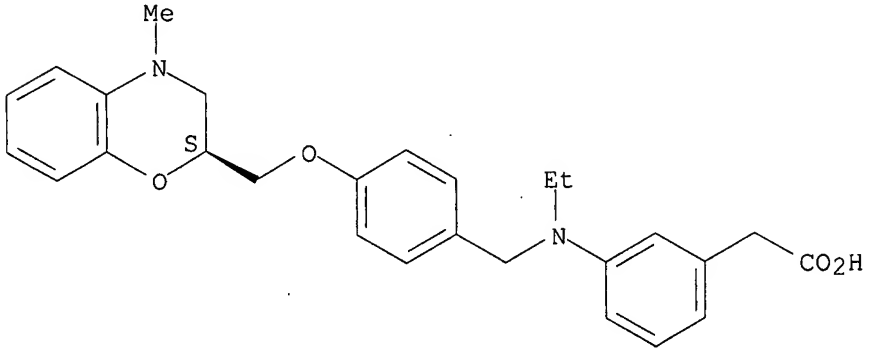
Absolute stereochemistry.

Updated Search



RN 603108-55-0 HCAPLUS
CN Benzeneacetic acid, 3-[[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]phenyl]methyl]ethylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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L3 3 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 15:00:40 ON 06 APR 2007
L4 1 S L3

FILE 'CAOLD' ENTERED AT 15:00:51 ON 06 APR 2007
L5 0 S L3

FILE 'REGISTRY' ENTERED AT 15:00:56 ON 06 APR 2007
L6 STRUCTURE UPLOADED
L7 0 S L6
L8 0 S L6 FULL

Updated Search

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Updated Search
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     FILE 'REGISTRY' ENTERED AT 15:00:56 ON 06 APR 2007
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L16          1 S L15 NOT L13
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L28          0 S L17 AND NAMBU, F?/AU

=> d l17, ibib abs hitstr, 1-18

L17  ANSWER 1 OF 18  HCAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2007:259556  HCAPLUS
DOCUMENT NUMBER:          146:316951
TITLE:                    Preparation of piperazinecarboxamides,
                          diazepanecarboxamides and their analogs as niacin
                          receptor agonists for the treatment of
                          atherosclerosis, dyslipidemia and diabetes
INVENTOR(S):              Colletti, Steven L.; Shen, Hong; Tata, James R.;
                          Szymonifka, Michael J.
PATENT ASSIGNEE(S):       Merck & Co., Inc., USA
SOURCE:                   PCT Int. Appl., 55pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:


Updated Search
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10572578

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007027532	A2	20070308	WO 2006-US33304	20060825

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-712275P P 20050829

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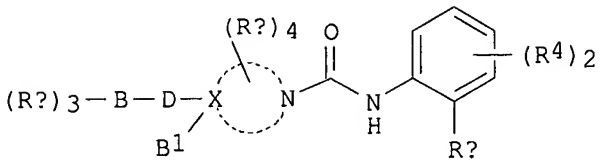

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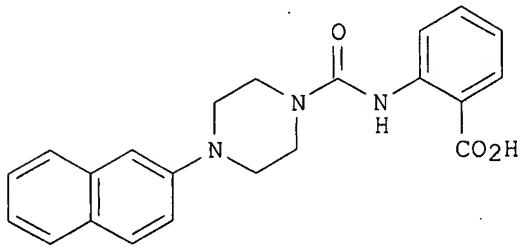


II

AB Title compds. I [wherein X = C or N; D = bond, O, CH2, CH2CH2 or CH2CH2CH2; B = (hetero)aryl; B' = H or absent; B and B' can be taken together to form a spiro ring while D = bond; Ra = H, halo, OH, etc.; Rb = H, halo, alkyl, etc.; Rc = COOH or tetrazol-5-yl; R4 = H, halo or (halo)methyl, with limitations] or pharmaceutically acceptable salts and solvates were prepared as niacin receptor agonists. Solid-phase synthesis of I such as II on Wang resin was disclosed. The invented compds. generally have EC50 in the range of 1 μM to 100 μM for niacin receptor in the binding assay. I are useful for the treatment of atherosclerosis, dyslipidemia, diabetes and other conditions.

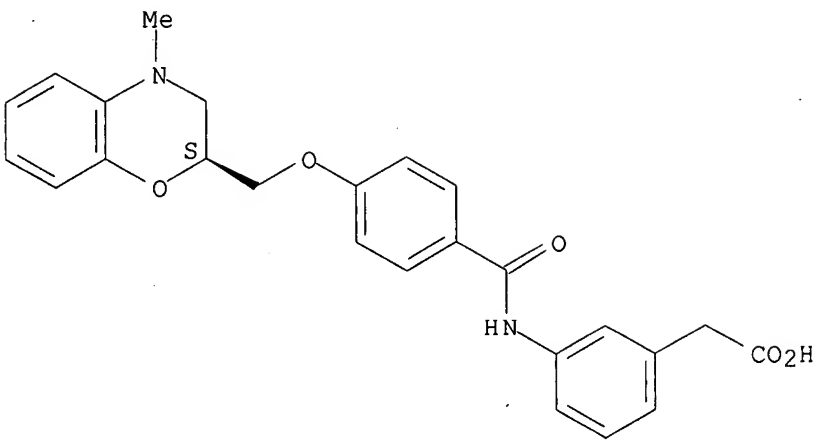
IT 603107-38-6 794535-33-4
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(co-drug; preparation of piperazinecarboxamides, diazepanecarboxamides and their analogs as niacin receptor agonists for treatment of atherosclerosis, dyslipidemia and diabetes)

RN 603107-38-6 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

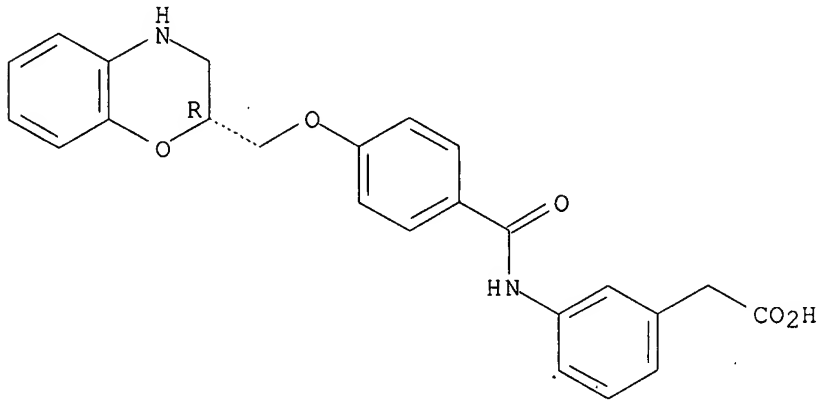
Updated Search

Absolute stereochemistry.



RN 794535-33-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2R)-3,4-dihydro-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1356948 HCAPLUS
DOCUMENT NUMBER: 146:100362
TITLE: Preparation of 2-acylaminocycloalkenecarboxylic acids derivatives as niacin receptor agonists
INVENTOR(S): Raghavan, Subharekha; Colletti, Steven L.; Ding, Fa-Xiang; Shen, Hong; Tata, James R.; Lins, Ashley Rouse; Smenton, Abigail Lee; Chen, Weichun; Schmidt, Darby Rye; Tria, George Scott
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 69pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English

Updated Search

10572578

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006293364	A1	20061228	US 2006-474646	20060626
WO 2007002557	A1	20070104	WO 2006-US24740	20060626

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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-694711P P 20050628
OTHER SOURCE(S): MARPAT 146:100362
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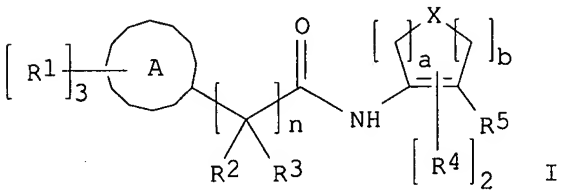

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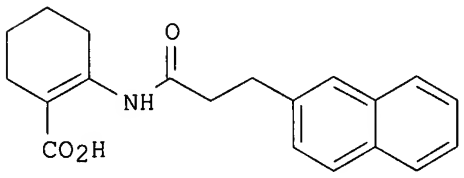


II

AB Title compds. I [X = CH2, O, S, etc.; a, b = 1-3 such as a + b = 2-4; ring A = aryl, heteroaryl, partially aromatic heterocyclic group, said heteroaryl and partially aromatic heterocyclic group containing at least one heteroatom selected from O, S, SO, etc., and optionally containing 1 other heteroatom selected from O and S, and optionally containing 1-3 addnl. N atoms, with up to 5 heteroatoms being present; R2, R3 = H, alkyl, haloalkyl, etc.; n = 1-5; R4 = H, halo, R6; R6 = alkyl optionally substituted with 1-3 groups, 0-3 of which are halo, and 0-1 of which are selected from the group consisting of O-alkyl, hydroxy, amino, etc.; R5 = -CO2H, tetrazol-5-yl, etc.; R1 = H, halo, hydroxy, etc.], pharmaceutically acceptable salts or solvates thereof were prepared For example, reaction of 3-(naphthalen-2-yl)propionic acid with methanesulfonyl chloride followed by in-situ treatment with Me 2-aminocyclohex-2-ene-1-carboxylate and hydrolysis using NaOH afforded compound II. The invented compds. generally

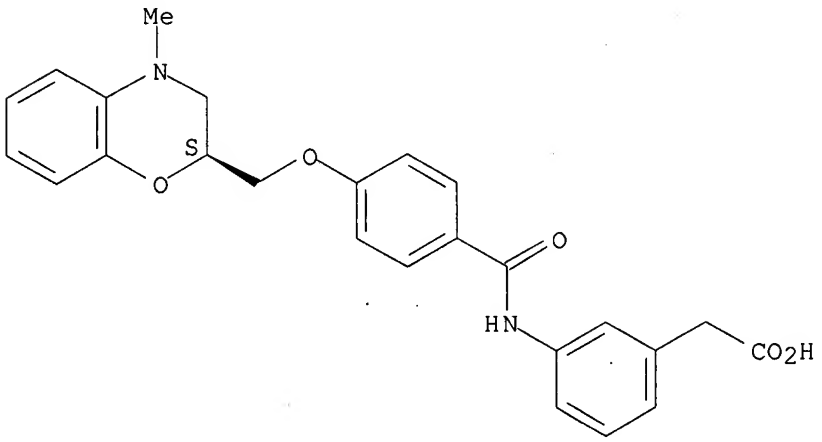
Updated Search

have an IC50 in the 3H-nicotinic acid competition binding assays within the range of 1 nM to about 25 μM, and have an EC50 in the functional in vitro GTPγS binding assays within the range of about 1-100 μM.

IT 603107-38-6 887146-38-5
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(medicaments with; preparation of 2-acylaminocycloalkenecarboxylic acids as niacin receptor agonists)

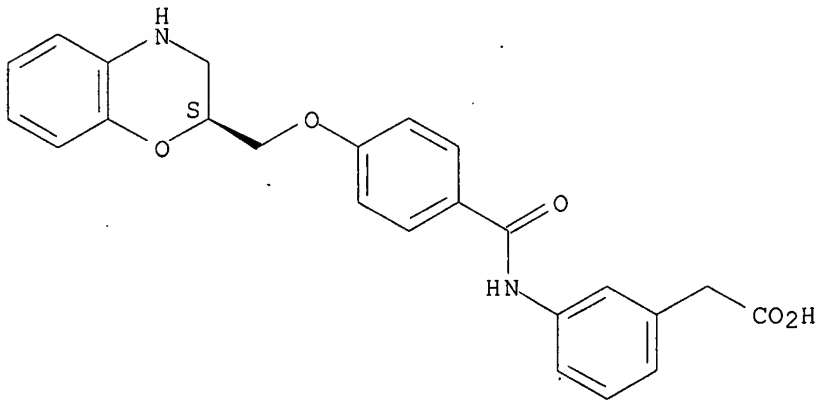
RN 603107-38-6 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 887146-38-5 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1124674 HCAPLUS
DOCUMENT NUMBER: 145:455008
TITLE: Preparation of pyrazole derivatives as Niacin receptor

Updated Search

10572578

agonists

INVENTOR(S): Imbriglio, Jason E.; Colletti, Steven L.; Tata, James R.; Liang, Rui; Raghavan, Subharekha; Schmidt, Darby R.; Smenton, Abigail R.; Chan, Sook Yee

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 83pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006113150	A1	20061026	WO 2006-US12876	20060407

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-670764P P 20050413
OTHER SOURCE(S): MARPAT 145:455008

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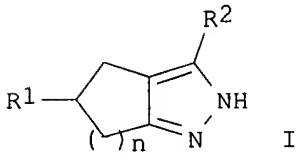

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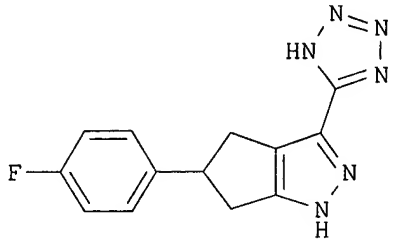


II

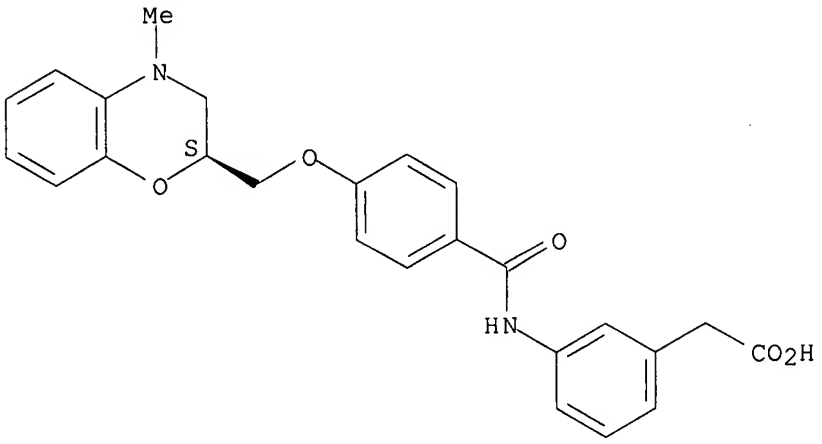
AB Title compds. represented by the formula I [wherein R1 = (un)substituted cyclohexyl, Ph or heteroaryl; R2 = tetrazol-5-yl, 2,4-dioxo-oxazol-5-yl or CO2R; R = H or alkyl; n = 1 or 2; and pharmaceutically acceptable salts or solvates thereof] were prepared as Niacin receptor agonists. For example, II was provided in a multi-step synthesis starting from 3-ethoxy cyclopentenone. Certain I an IC50 in the niacin binding assay within the range of about 0.010-50 μM, and have an EC50 in the functional GTPγS binding assay within the range of about 0.010-100 1M. Thus, I and their pharmaceutical compns. are useful as Niacin receptor agonists for the treatment of dyslipidemias (no data).

IT 603107-38-6P 794535-33-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

Updated Search

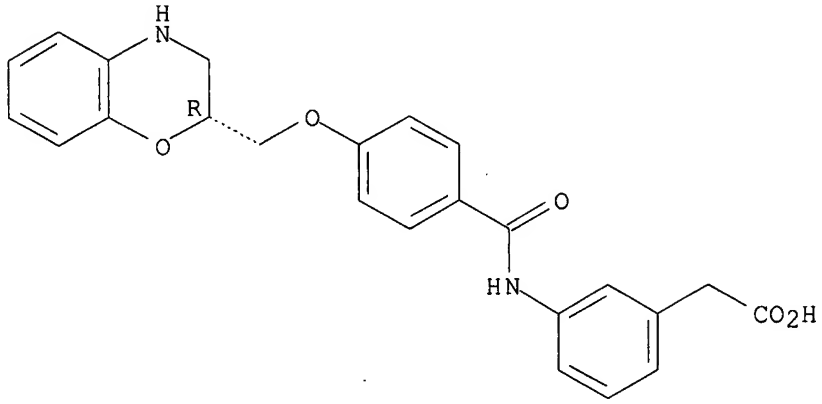
(Uses)
(preparation of pyrazole derivs. as Niacin receptor agonists)
RN 603107-38-6 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 794535-33-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2R)-3,4-dihydro-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:635044 HCAPLUS
DOCUMENT NUMBER: 145:103670
TITLE: Fused pyrazole derivatives and their preparation, pharmaceutical compositions, and methods for treatment of metabolic-related disorders
INVENTOR(S): Boatman, Douglas P.; Schrader, Thomas O.; Semple,

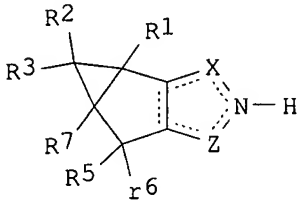
Updated Search

10572578

Graeme; Skinner, Philip J.; Jung, Jae-Kyu
PATENT ASSIGNEE(S): Arena Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 170 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006069242	A2	20060629	WO 2005-US46599	20051222
WO 2006069242	A3	20060831		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
US 2006205955	A1	20060914	US 2005-315753	20051222
US 2007073062	A1	20070329	US 2006-601184	20061117
PRIORITY APPLN. INFO.:			US 2004-638668P	P 20041223
			US 2005-676521P	P 20050429
			US 2005-315753	A1 20051222

OTHER SOURCE(S): MARPAT 145:103670
GI



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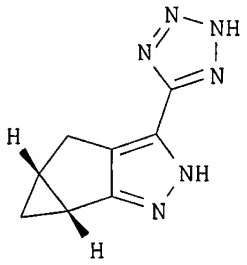


II

AB The invention relates to certain fused pyrazole derivs. of formula I, and pharmaceutically acceptable salts thereof, which exhibit useful pharmacol. properties, for example, as agonists for the RUP25 receptor. Compds. of formula I wherein X is N, and Z is CR7, or X is CR7 and Z is N; one dotted lines are single and double bonds such that the ring containing X and Z is a pyrazole ring; R1 - R6 are independently H, C1-6 acyl(oxy), C2-6 alkenyl, C1-6 alkoxy, C1-6 alkyl(amino), C1-6 alkyl(thio)carboxamide, C2-6 alkynyl, etc.; R7 is carbo-C1-6 alkoxy, carboxy, or tetrazol-5-yl; and their pharmaceutically acceptable salts, hydrates, or solvates thereof are claimed. Also provided by the invention are pharmaceutical compns. containing compds. of the invention, and methods of using the compds. and compns. of the invention in the treatment of metabolic-related disorders, including dyslipidemia, atherosclerosis, coronary heart disease, insulin resistance,

Updated Search

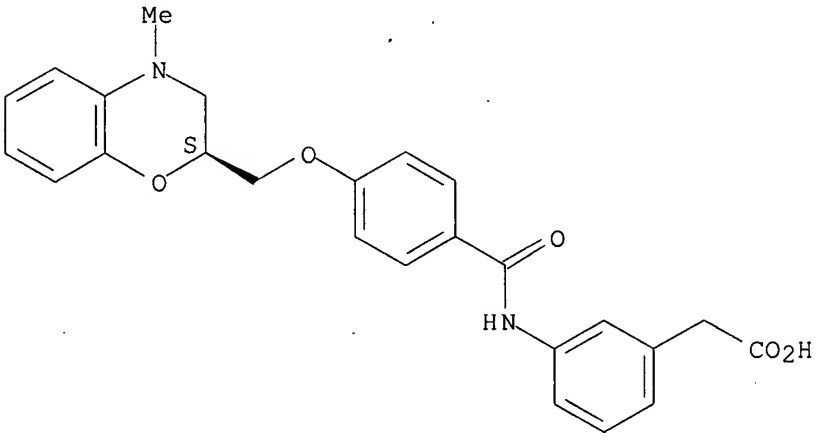
type 2 diabetes, Syndrome-X and the like. In addition, the invention also provides for the use of the compds. of the invention in combination with other active agents such as those belonging to the class of α-glucosidase inhibitors, aldose reductase inhibitors, biguanides, HMG-CoA reductase inhibitors, squalene synthesis inhibitors, fibrates, LDL catabolism enhancers, angiotensin converting enzyme (ACE) inhibitors, insulin secretion enhancers, DP receptor antagonists, and the like. Example compound II was prepared by cyclization of (R)-2-(3-butenyl)oxirane; the resulting bicyclo[3.2.1]hexan-2-ol underwent oxidation of give bicyclo[3.2.1]hexane-2-one, which underwent cyclization with di-Et oxalate and hydrazine to give 1a,2,5,5a-tetrahydro-1H-2,3-diazacyclopropa[a]pentalene-4-carboxylic acid Et ester, which underwent amidation with ammonium hydroxide to give the corresponding amide, which benzylation with benzyl bromide followed by dehydration to give 2-benzyl-1a,2,5,5a-tetrahydro-1H-2,3-diazacyclopropa[a]pentalene-4-carbonitrile, which reacted with sodium azide to give 2-Benzyl-4-(2H-tetrazol-5-yl)-1a,2,5,5a-tetrahydro-2,3-diazacyclopropa[a]pentalene, which underwent debenzylation to give example compound II. All the invention compds. were evaluated for their antihyperglycemic activity, and 35S-GTPγS, human RUP25, and 3H-nicotinic acid receptor binding affinities. Certain compds. were determined to have an EC50 value in the cAMP whole cell method of about 25 μM or less. From the in vitro GTPγS binding assay, it was determined that tested compds. exhibited EC50 values in the range of about 1-100 μM, and the best compds. showed an EC50 value of less than about 1 μM. Certain tested compds. have an EC50 in the 3H-nicotinic acid binding competition assay, in the range of 1 to 100 μM , and the most favorable compds. exhibited an EC50 value of less than about 1 μM.

IT 603107-38-6P 794535-33-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of fused pyrazole derivs. and methods for treatment of metabolic-related disorders)

RN 603107-38-6 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



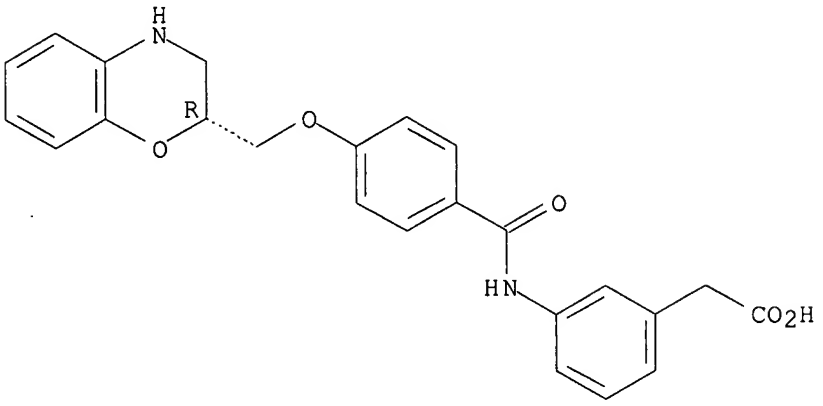
RN 794535-33-4 HCAPLUS

Updated Search

10572578

CN Benzeneacetic acid, 3-[[4-[[(2R)-3,4-dihydro-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



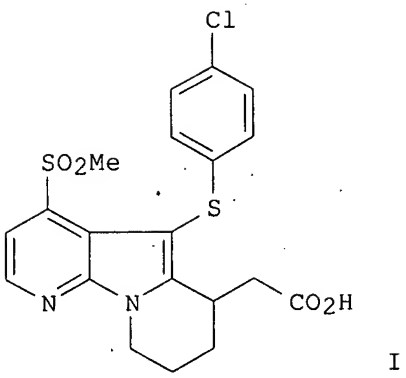
L17 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:471897 HCAPLUS
DOCUMENT NUMBER: 144:488635
TITLE: Preparation of compounds such as pyridoindolizine and indole derivatives as prostaglandin D2 antagonists for treating pathological blushing
INVENTOR(S): Tobert, Jonathan A.; Lai, Eseng
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 40 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006052798	A2	20060518	WO 2005-US40117	20051107
WO 2006052798	A3	20070111		
WO 2006052798	B1	20070222		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-625823P P 20041108
GI

Updated Search



I

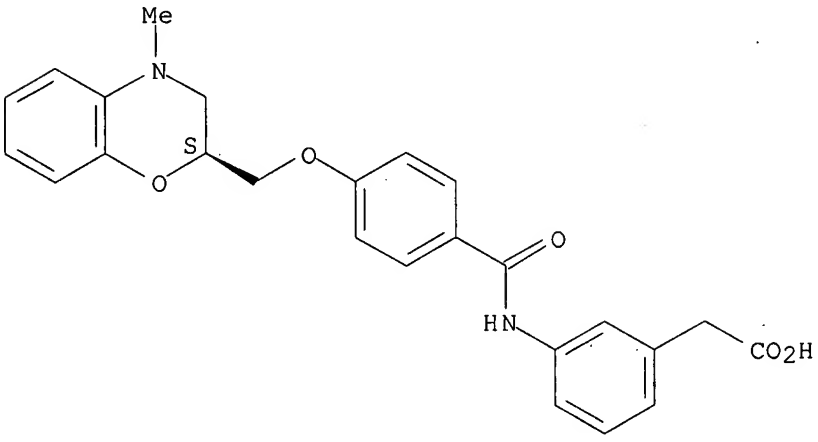
AB A method of treating pathol. blushing is disclosed wherein the patient is administered a DP (prostaglandin D2) receptor antagonist. E.g, I was prepared by a series of reactions starting from 4-chloronicotinaldehyde. The compds. prepared function as selective DP antagonists and demonstrate an affinity for DP that is at least about 10 times higher than the affinity for CRTH2 receptors.

IT 603107-38-6P 887146-38-5P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of compds. such as pyridoindolizine and indole derivs. as prostaglandin D2 antagonists for treating pathol. blushing)

RN 603107-38-6 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



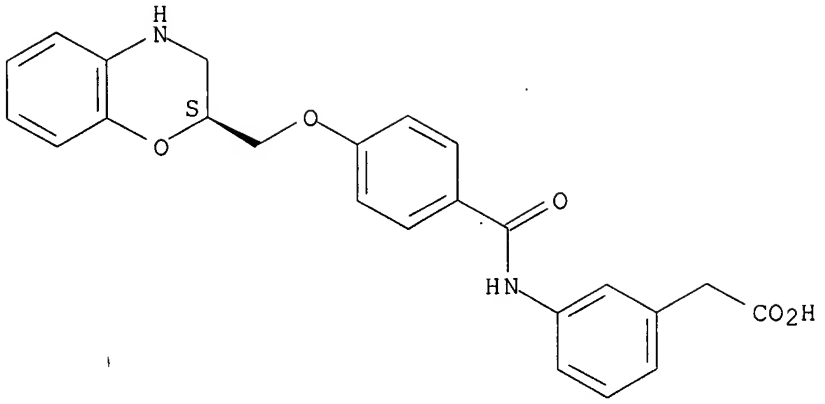
RN 887146-38-5 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Updated Search

10572578



L17 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:212213 HCAPLUS
DOCUMENT NUMBER: 144:292761
TITLE: Preparation of 3-(2H-tetrazol-5-yl)-1,4,5,6-tetrahydrocyclopentapyrazole as nicotinic agonist and pyridoindolizine derivatives as DP receptor antagonists , and their combination useful for treating atherosclerosis, dyslipidemias and related conditions
INVENTOR(S): Waters, M. Gerard; Turner, Mervyn
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006026273	A2	20060309	WO 2005-US30001	20050824
WO 2006026273	A3	20060908		

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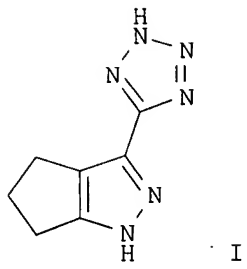
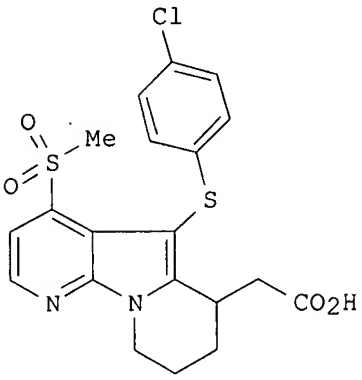
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-604443P P 20040825
GI

Updated Search



I



II

AB The invention is related to a method of treating atherosclerosis, dyslipidemia and related conditions wherein a nicotinic acid receptor partial/agonist I, or one of its pharmaceutically acceptable salts or solvates, is administered to a human patient in combination with a DP receptor antagonist, e.g. II, in amts. that are effective for treatment in the absence of substantial flushing. The invention is also related to the preparation of tetrazole I and DP antagonists. Thus, I was prepared by reaction of cyclopentanone with diethylmalonate (no data for the intermediate), followed by cyclization with hydrazine hydrochloride, amidation of the ester with methanolic ammonia, dehydration of the amide, and cyclization of the nitrile with NaN3. An 11-step synthesis was given for pyridoindolizine II (no data for the intermediates). II, and its derivs., having a binding affinity (Ki) for CRTH2 of about ≥ 0.5 μM, and a selectivity for the DP receptor over CRTH2 of at least about 10 fold, are useful to inhibit the flushing effect seen when tetrazole I or its pharmaceutically acceptable salts or solvates are administered alone.

IT 603107-38-6P 794535-33-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(DP receptor antagonist; preparation of a nicotinic agonist and DP receptor antagonists, and their combination useful for treating atherosclerosis, dyslipidemias and related conditions)

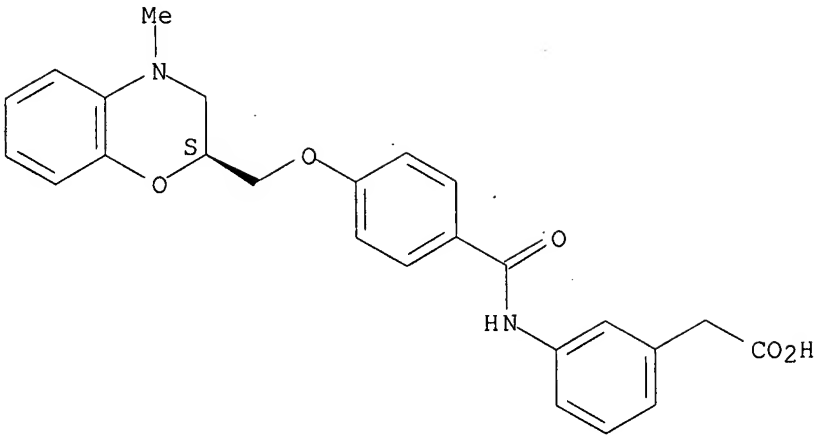
RN 603107-38-6 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

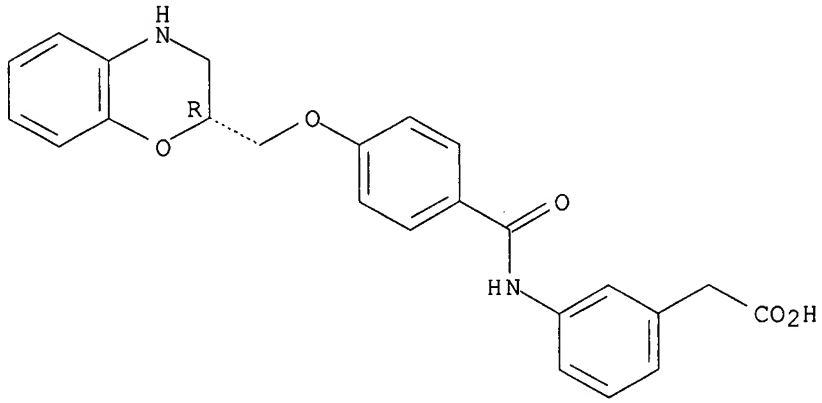
Updated Search

10572578



RN 794535-33-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2R)-3,4-dihydro-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:570879 HCAPLUS
DOCUMENT NUMBER: 143:97370
TITLE: Preparation of triazolylsulphanyl phenyl ethers as modulators of PPAR receptors
INVENTOR(S): Diaz, Philippe; Raffin, Catherine
PATENT ASSIGNEE(S): Galderma Research & Development, S.N.C., Fr.
SOURCE: PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005058844	A2	20050630	WO 2004-EP14810	20041208

Updated Search

10572578

WO 2005058844				A3	20050929										
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	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
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	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
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RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
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CA 2545767				A1	20050630		CA 2004-2545767							20041208		
EP 1694669				A2	20060830		EP 2004-804396							20041208		
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US 2007054907				A1	20070308		US 2006-450392							20060612		
PRIORITY APPLN. INFO.:							FR 2003-14535						A	20031211		
							US 2003-530234P						P	20031218		
							WO 2004-EP14810						W	20041208		

OTHER SOURCE(S): MARPAT 143:97370
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

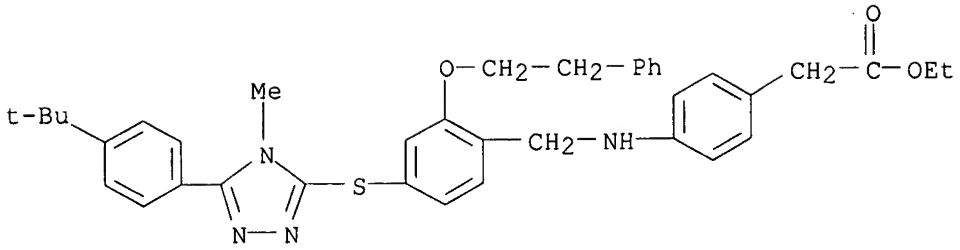
AB Title compds. I [R1 = H, alkyl, aryl, etc.; R2 = H, aryl, (un)substituted alkyl, etc.; R3 = alkyl, aralkyl; R4 = OH, alkoxy, NR6R7; R5 = H, halo, alkoxy, etc.; R6 and R7 independently = H, alkyl or together with the nitrogen atom form a morpholino, piperidino or pyrrolidino group; n = 0-2; m = 0-1; X = S, Se, O, etc.] and their pharmaceutically acceptable salts, are prepared and disclosed as modulators of PPAR receptors. Thus, e.g., II was prepared by amidation of (4-{4-[5-(4-tert-butylphenyl)-4-methyl-4H-[1,2,4]-triazol-3-ylsulphanyl]-2-heptyloxybenzylamino}phenyl)acetic acid (preparation given) with n-hexylamine. The transactivation capability of I was evaluated using luminescence assay and it was revealed that selected compds. of the invention displayed a Kd app value against PPARγ in the range of 15-60 nM. I as modulators of PPAR receptors should prove useful in the treatment of dermatol. conditions, such as but not limited to, acne vulgaris, ichthyosis, and skin aging. Cosmetic and pharmaceutical compns. comprising I are disclosed.

IT 854028-54-9P 854028-56-1P 854028-62-9P
854028-64-1P 854028-70-9P 854028-72-1P
854028-74-3P 854028-76-5P 854028-82-3P
854028-84-5P 854028-90-3P 854028-92-5P
RL: COS (Cosmetic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of triazolylsulphanyl Ph ethers as modulators of PPAR receptors)

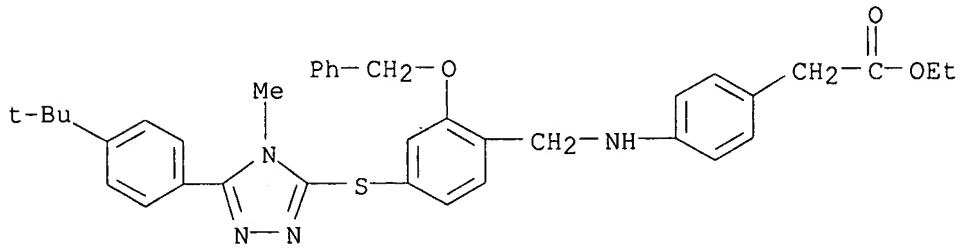
RN 854028-54-9 HCAPLUS

CN Benzeneacetic acid, 4-[[[4-[[5-[4-(1,1-dimethylethyl)phenyl]-4-methyl-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

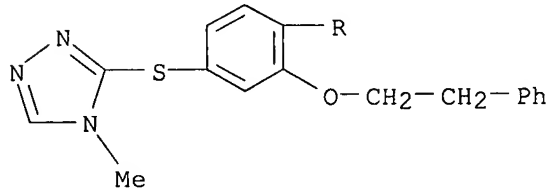
Updated Search

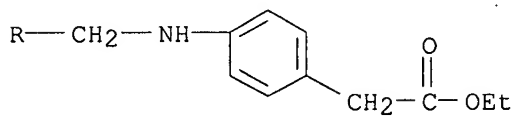


RN 854028-56-1 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[4-(1,1-dimethylethyl)phenyl]-4-methyl-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



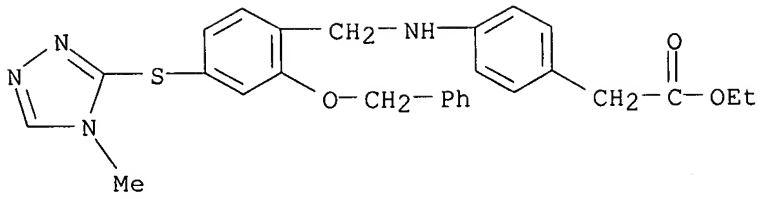
RN 854028-62-9 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[(4-methyl-4H-1,2,4-triazol-3-yl)thio]-2-(2-phenylethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



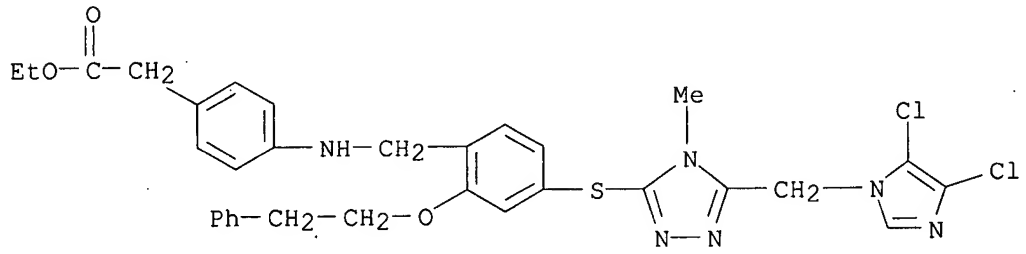


RN 854028-64-1 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[(4-methyl-4H-1,2,4-triazol-3-yl)thio]-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

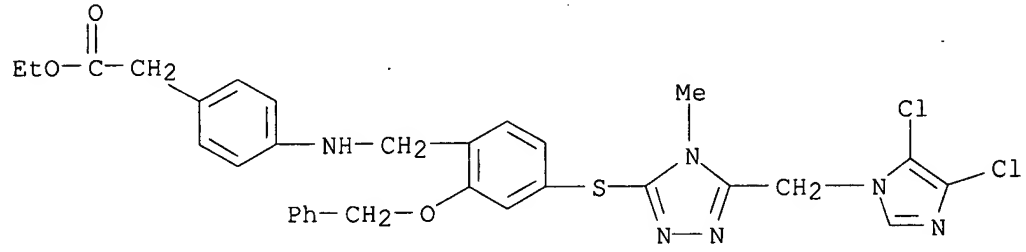
Updated Search



RN 854028-70-9 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[(4,5-dichloro-1H-imidazol-1-yl)methyl]-4-methyl-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

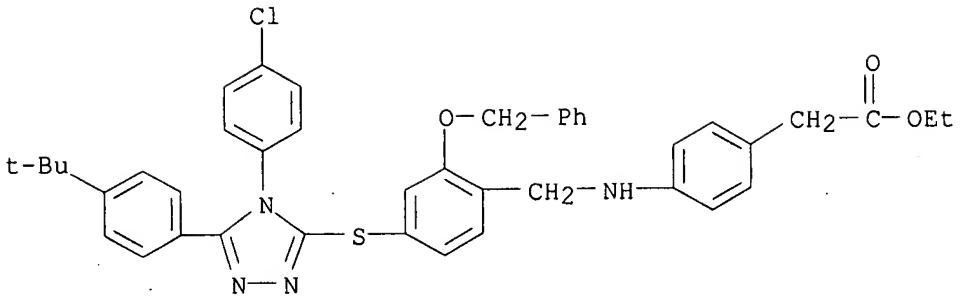


RN 854028-72-1 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[(4,5-dichloro-1H-imidazol-1-yl)methyl]-4-methyl-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

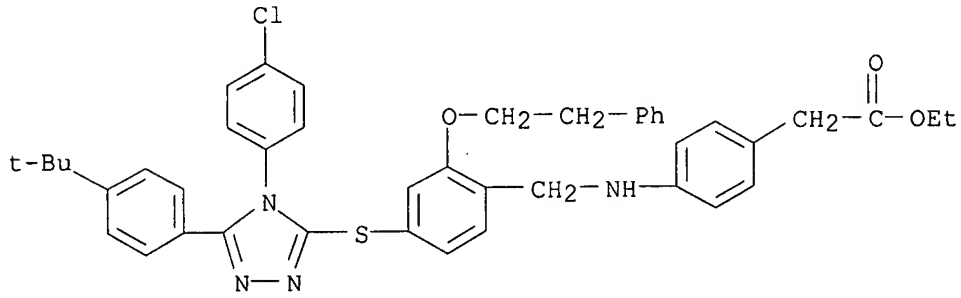


RN 854028-74-3 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-(4-chlorophenyl)-5-[4-(1,1-dimethylethyl)phenyl]-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

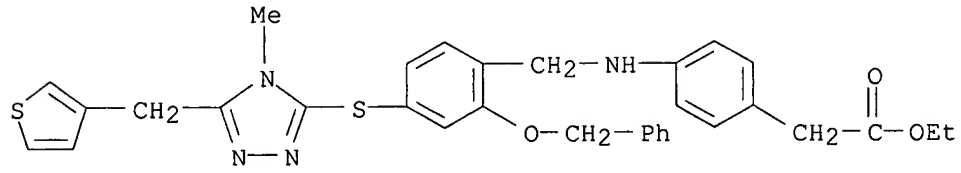
Updated Search



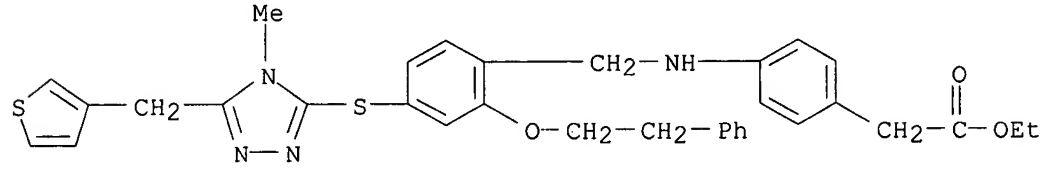
RN 854028-76-5 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-(4-chlorophenyl)-5-[4-(1,1-dimethylethyl)phenyl]-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 854028-82-3 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-methyl-5-(3-thienylmethyl)-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



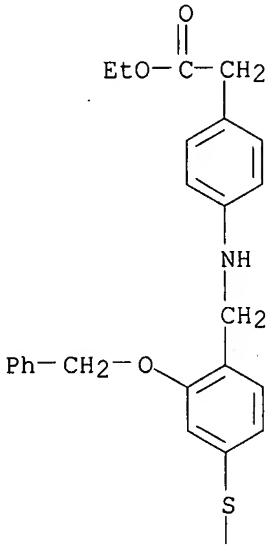
RN 854028-84-5 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-methyl-5-(3-thienylmethyl)-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



Updated Search

RN 854028-90-3 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[[(2,3-dihydro-7-methyl-1H-inden-4-yl)oxy]methyl]-4-phenyl-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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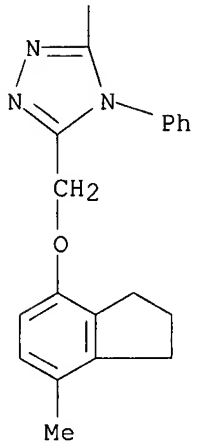
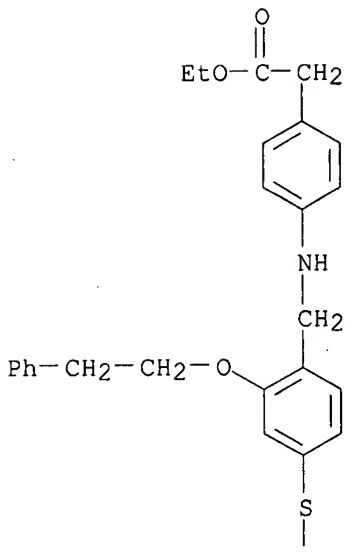


RN 854028-92-5 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[[(2,3-dihydro-7-methyl-1H-inden-4-yl)oxy]methyl]-4-phenyl-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Updated Search

PAGE 1-A



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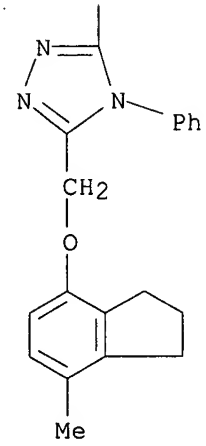

IT 854028-53-8P 854028-55-0P 854028-61-8P
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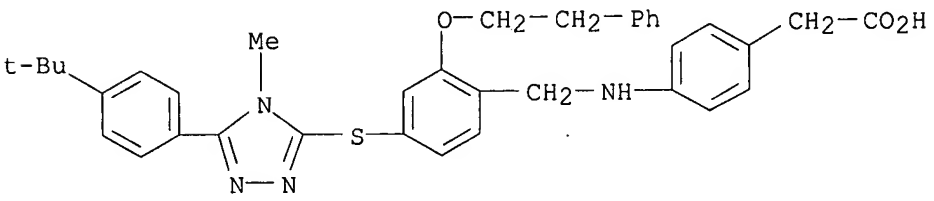
RL: COS (Cosmetic use); CPN (Combinatorial preparation); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); CMBI (Combinatorial study); PREP (Preparation); USES (Uses)
(preparation of triazolylsulphanyl Ph ethers as modulators of PPAR receptors

Updated Search

via solid phase parallel synthesis employing lantern technol.)

RN 854028-53-8 HCAPLUS

CN Benzeneacetic acid, 4-[[[4-[[5-[4-(1,1-dimethylethyl)phenyl]-4-methyl-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)



RN 854028-55-0 HCAPLUS

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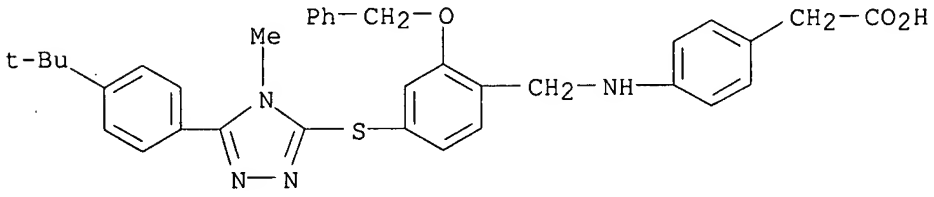

RN 854028-61-8 HCAPLUS

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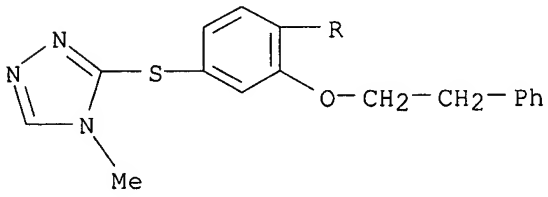
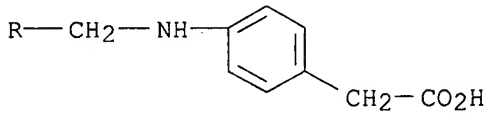
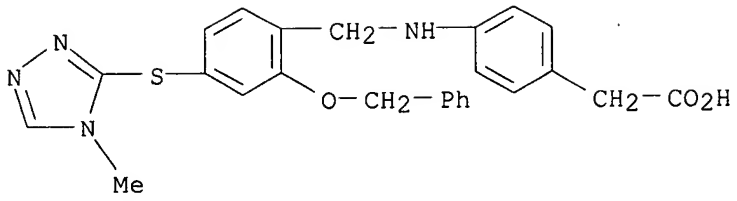




RN 854028-63-0 HCAPLUS

CN Benzeneacetic acid, 4-[[[4-[(4-methyl-4H-1,2,4-triazol-3-yl)thio]-2-(phenylmethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Updated Search



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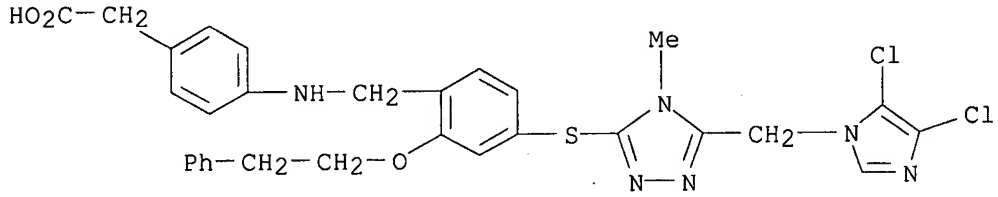

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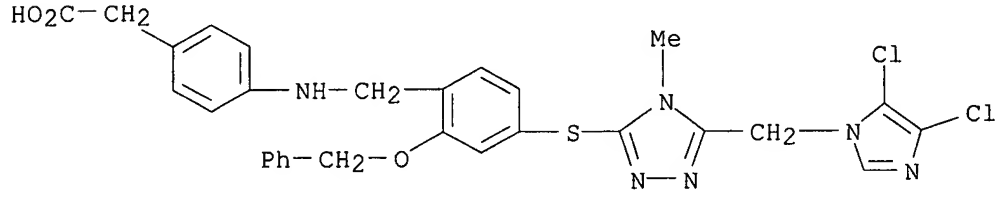

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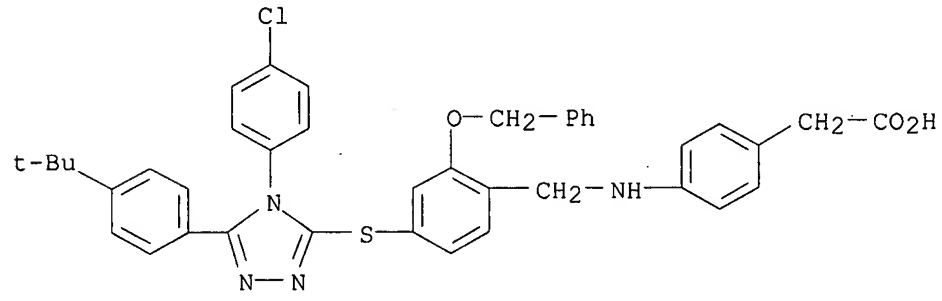

RN 854028-75-4 HCAPLUS

Updated Search

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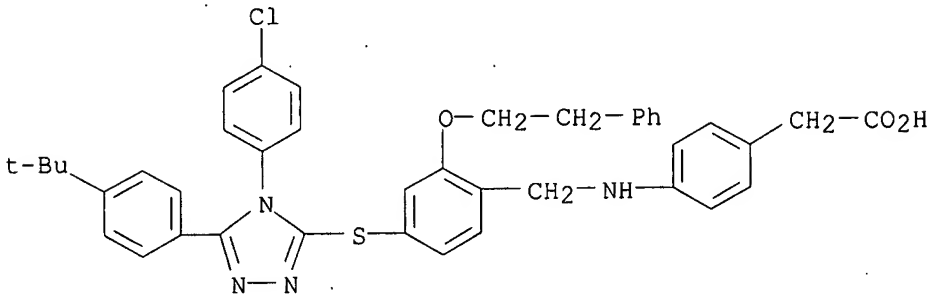

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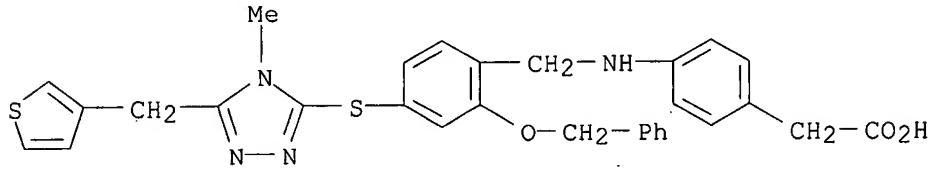

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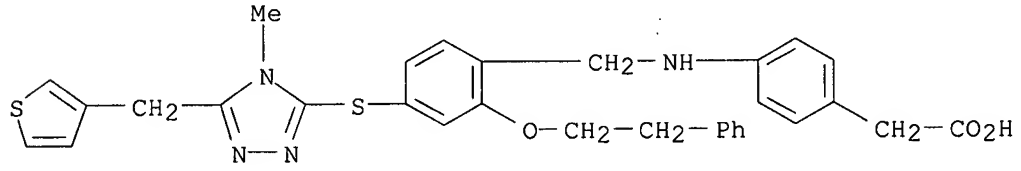

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Updated Search

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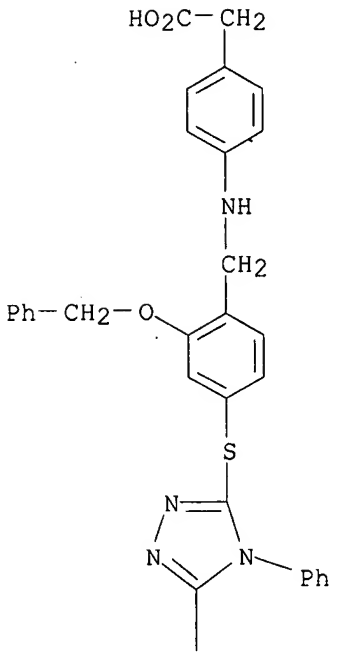

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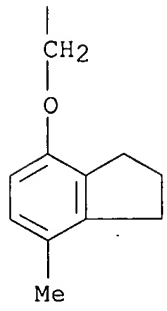

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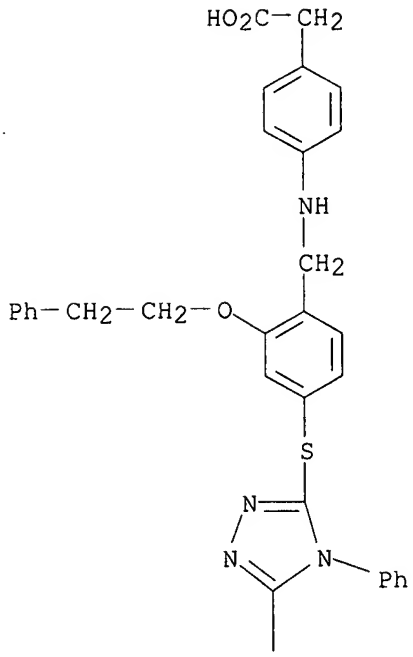
Updated Search

PAGE 1-A



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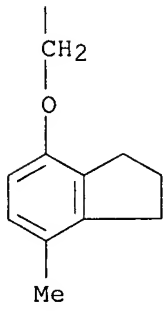

L17 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:521779 HCAPLUS
DOCUMENT NUMBER: 143:59985
TITLE: Preparation of triazoles as PPAR modulators for pharmaceuticals and cosmetics
INVENTOR(S): Diaz, Philippe; Raffin, Catherine
PATENT ASSIGNEE(S): Galderma Research & Development, Fr.
SOURCE: Fr. Demande, 49 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

Updated Search

10572578

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2863610	A1	20050617	FR 2003-14535	20031211
FR 2863610	B1	20060120		
CA 2545767	A1	20050630	CA 2004-2545767	20041208
WO 2005058844	A2	20050630	WO 2004-EP14810	20041208
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OTHER SOURCE(S): MARPAT 143:59985

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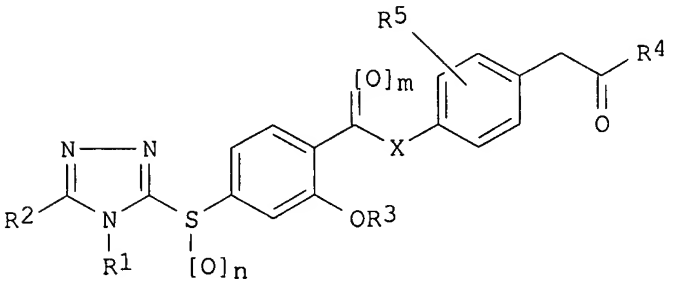

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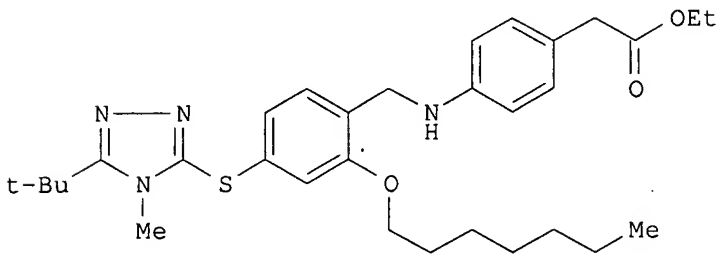

II

AB Title compds. I [wherein R1 = H, ar/alkyl, hetero/aryl; R2 = H, alkyl, aryl, etc.; X = S, Se, O, NH and derivs.; R3 = ar/alkyl; R4 = OH, alkoxy, NH2 and derivs.; R5 = H, halo, alkyl, alkoxy, OH; n = 0-2; m = 0-1; when X

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= S, Se and m = 0, then n = 0; their optical and/or geometrical isomers, their mixts., tautomers and N-oxides] were prepared as PPAR modulators for pharmaceutical or cosmetic uses. Two synthetic examples, 10 formulations and 57 claimed compds. are given. A parallel synthesis is given for several invention compds. For example, S-alkylation of 5-(4-tert-butylphenyl)-4-methyl-4H-[1,2,4]triazole-3-thiol with Et 2-[4-(2-heptyloxy-4-iodobenzylamino)phenyl]acetate (preparation given) gave II in 90% yield. I showed PPARγ activity with Kd apparent of 15 nM in a crossover-curve PPAR activation test. For example, a tablet formulation contains triazole (II) 0.001, starch 0.114, dicalcium phosphate 0.020, silica 0.020, lactose 0.030, talc 0.010, and Mg stearate 0.005 g.

IT 854028-53-8P, [4-[[4-[[5-(4-tert-Butylphenyl)-4-methyl-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-phenethyloxybenzyl]amino]phenyl]acetic acid 854028-54-9P, Ethyl 2-[4-[[4-[[5-(4-tert-Butylphenyl)-4-methyl-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-phenethyloxybenzyl]amino]phenyl]acetate 854028-55-0P, [4-[[2-Benzyloxy-4-[[5-(4-tert-butylphenyl)-4-methyl-4H-[1,2,4]triazol-3-yl]sulfanyl]benzyl]amino]phenyl]acetic acid 854028-56-1P, Ethyl 2-[4-[[4-[[5-(4-tert-Butylphenyl)-4-methyl-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-benzyloxybenzyl]amino]phenyl]acetate 854028-61-8P, [4-[[4-[(4-Methyl-4H-[1,2,4]triazol-3-yl)sulfanyl]-2-phenethyloxybenzyl]amino]phenyl]acetic acid 854028-62-9P, Ethyl 2-[4-[[4-[(4-Methyl-4H-[1,2,4]triazol-3-yl)sulfanyl]-2-phenethyloxybenzyl]amino]phenyl]acetate 854028-63-0P, [4-[[4-[(4-Methyl-4H-[1,2,4]triazol-3-yl)sulfanyl]-2-benzyloxybenzyl]amino]phenyl]acetic acid 854028-64-1P, Ethyl 2-[4-[[4-[(4-methyl-4H-[1,2,4]triazol-3-yl)sulfanyl]-2-benzyloxybenzyl]amino]phenyl]acetate 854028-69-6P, [4-[[4-[[5-(4,5-Dichloroimidazol-1-ylmethyl)-4-methyl-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-phenethyloxybenzyl]amino]phenyl]acetic acid 854028-70-9P, Ethyl 2-[4-[[4-[[5-(4,5-Dichloroimidazol-1-ylmethyl)-4-methyl-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-phenethyloxybenzyl]amino]phenyl]acetate 854028-71-0P, [4-[[4-[[5-(4,5-Dichloroimidazol-1-ylmethyl)-4-methyl-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-benzyloxybenzyl]amino]phenyl]acetic acid 854028-72-1P, Ethyl 2-[4-[[4-[[5-(4,5-Dichloroimidazol-1-ylmethyl)-4-methyl-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-benzyloxybenzyl]amino]phenyl]acetate 854028-73-2P, [4-[[4-[[5-(4-tert-Butylphenyl)-4-(4-chlorophenyl)-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-benzyloxybenzyl]amino]phenyl]acetic acid 854028-74-3P, Ethyl 2-[4-[[4-[[5-(4-tert-Butylphenyl)-4-(4-chlorophenyl)-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-benzyloxybenzyl]amino]phenyl]acetate 854028-75-4P, [4-[[4-[[5-(4-tert-Butylphenyl)-4-(4-chlorophenyl)-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-phenethyloxybenzyl]amino]phenyl]acetic acid 854028-76-5P, Ethyl 2-[4-[[4-[[5-(4-tert-Butylphenyl)-4-(4-chlorophenyl)-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-phenethyloxybenzyl]amino]phenyl]acetate 854028-81-2P, [4-[[4-[[4-Methyl-5-[(thiophen-3-yl)methyl]-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-benzyloxybenzyl]amino]phenyl]acetic acid 854028-82-3P, Ethyl 2-[4-[[4-[[4-Methyl-5-[(thiophen-3-yl)methyl]-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-benzyloxybenzyl]amino]phenyl]acetate 854028-83-4P, [4-[[4-[[4-Methyl-5-[(thiophen-3-yl)methyl]-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-phenethyloxybenzyl]amino]phenyl]acetic acid 854028-84-5P, Ethyl 2-[4-[[4-[[4-Methyl-5-[(thiophen-3-yl)methyl]-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-phenethyloxybenzyl]amino]phenyl]acetate 854028-89-0P, [4-[[4-[[5-[[(7-Methylindan-4-yl)oxy]methyl]-4-phenyl-4H-[1,2,4]triazol-3-yl]sulfanyl]-2-benzyloxybenzyl]amino]phenyl]acetic acid 854028-90-3P, Ethyl 2-[4-[[4-[[5-[[(7-Methylindan-4-yl)oxy]methyl]-

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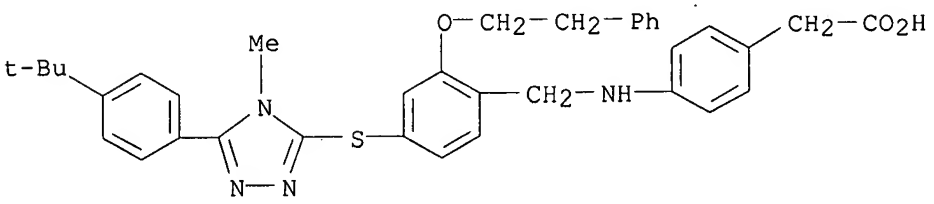
RL: COS (Cosmetic use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(PPAR modulator; preparation of triazoles as PPAR modulators for pharmaceuticals and cosmetics)

RN 854028-53-8 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[4-(1,1-dimethylethyl)phenyl]-4-methyl-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)



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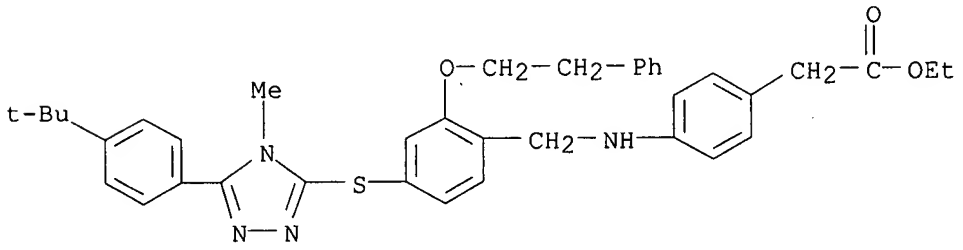

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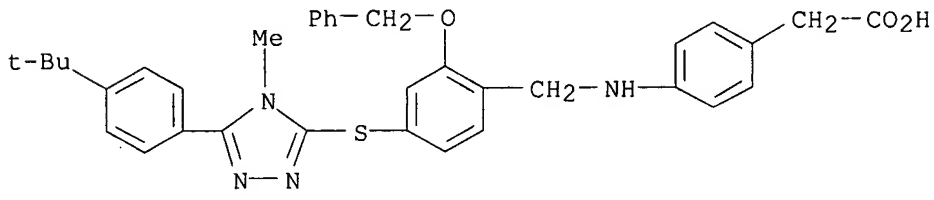
CN Benzeneacetic acid, 4-[[[4-[[5-[4-(1,1-dimethylethyl)phenyl]-4-methyl-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)



RN 854028-56-1 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[4-(1,1-dimethylethyl)phenyl]-4-methyl-4H-

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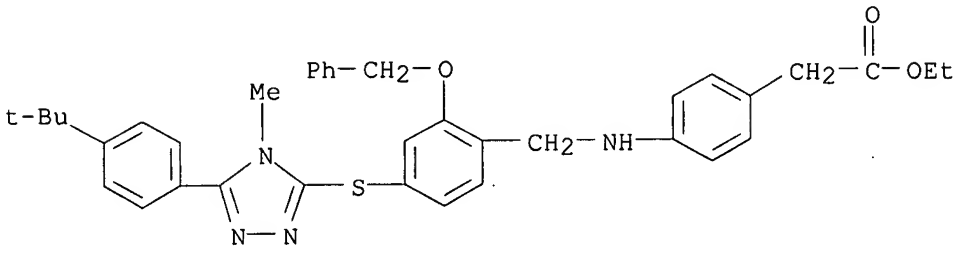
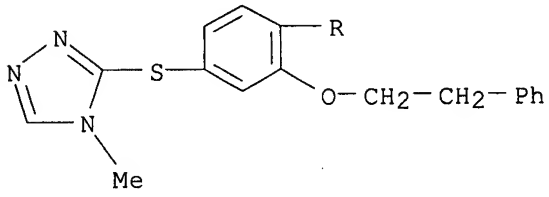
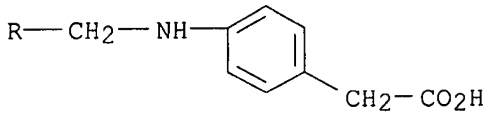


RN 854028-61-8 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[(4-methyl-4H-1,2,4-triazol-3-yl)thio]-2-(2-phenylethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)





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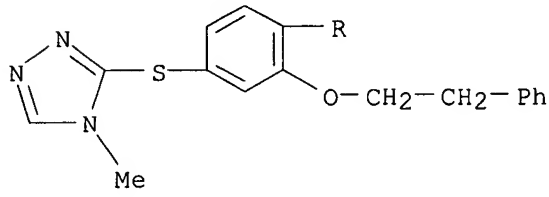
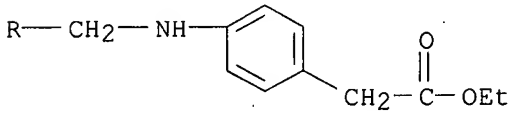
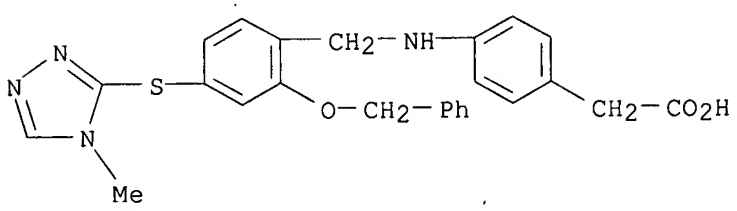




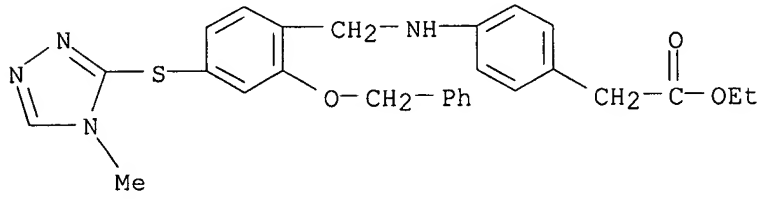
RN 854028-63-0 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[(4-methyl-4H-1,2,4-triazol-3-yl)thio]-2-

Updated Search

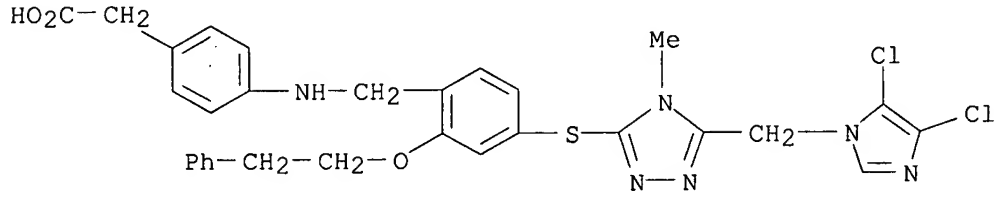
(phenylmethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)



RN 854028-64-1 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[(4-methyl-4H-1,2,4-triazol-3-yl)thio]-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 854028-69-6 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[(4,5-dichloro-1H-imidazol-1-yl)methyl]-4-methyl-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)



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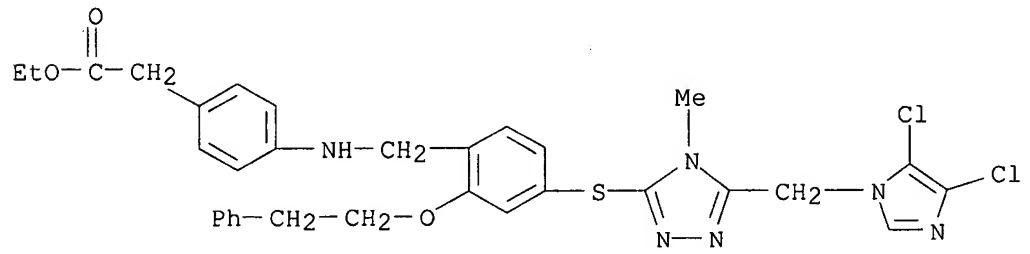
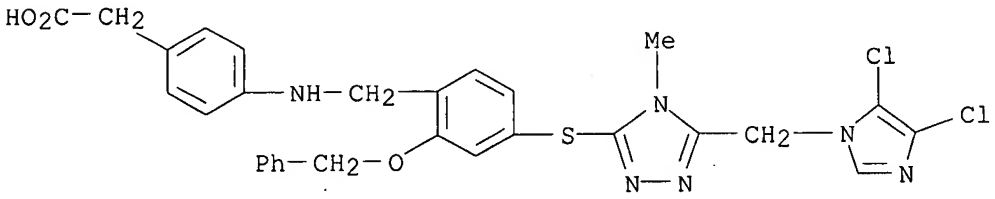


RN 854028-71-0 HCAPLUS

Updated Search

10572578

CN Benzeneacetic acid, 4-[[[4-[[5-[(4,5-dichloro-1H-imidazol-1-yl)methyl]-4-methyl-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)



RN 854028-72-1 HCAPLUS
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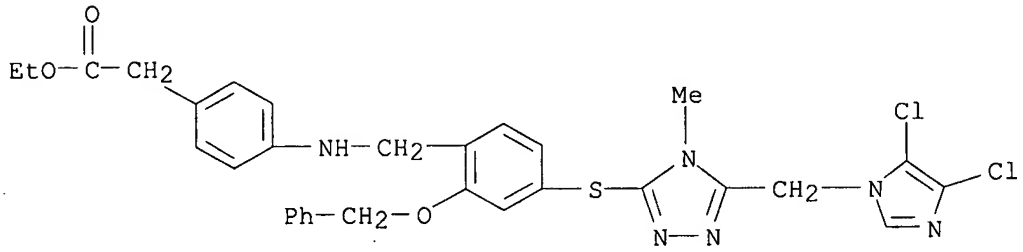
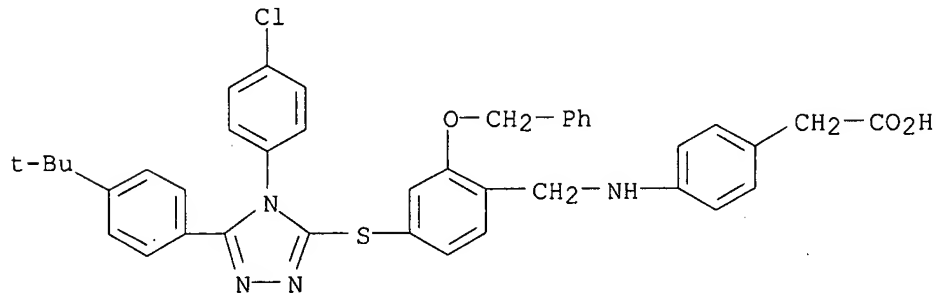
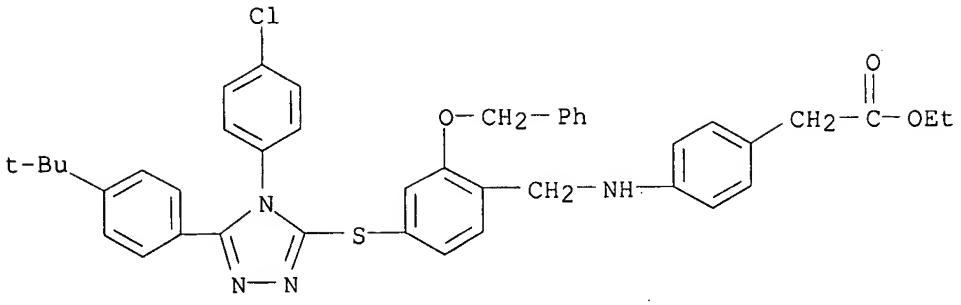


RN 854028-73-2 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-(4-chlorophenyl)-5-[4-(1,1-dimethylethyl)phenyl]-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

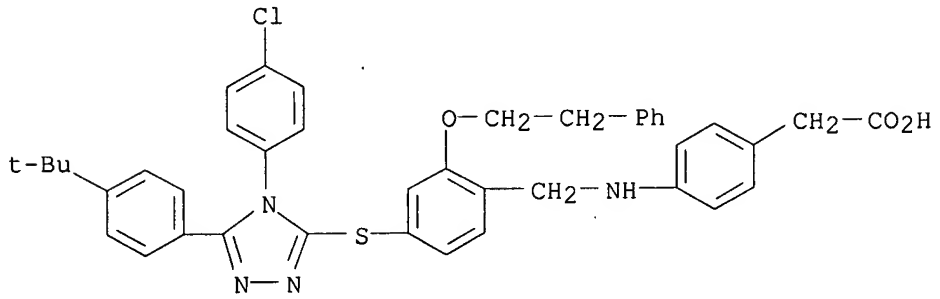


RN 854028-74-3 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-(4-chlorophenyl)-5-[4-(1,1-dimethylethyl)phenyl]-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

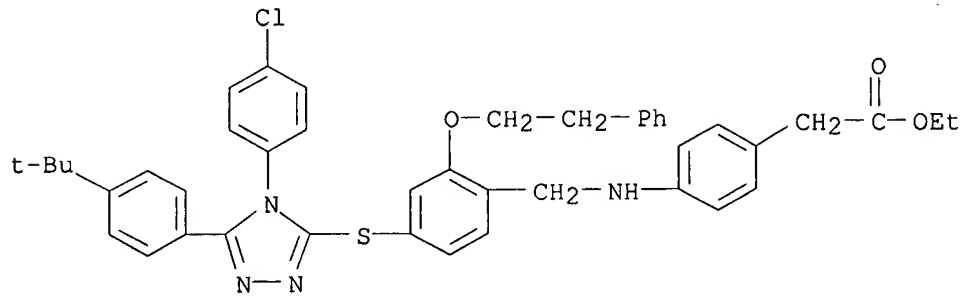
Updated Search



RN 854028-75-4 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-(4-chlorophenyl)-5-[4-(1,1-dimethylethyl)phenyl]-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)



RN 854028-76-5 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-(4-chlorophenyl)-5-[4-(1,1-dimethylethyl)phenyl]-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



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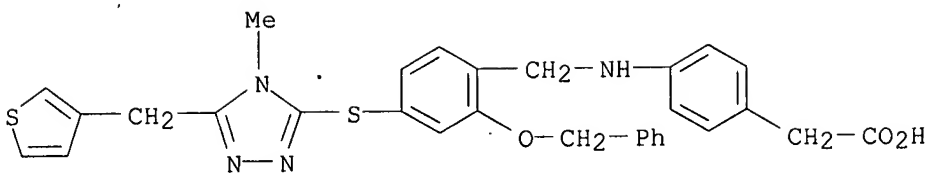
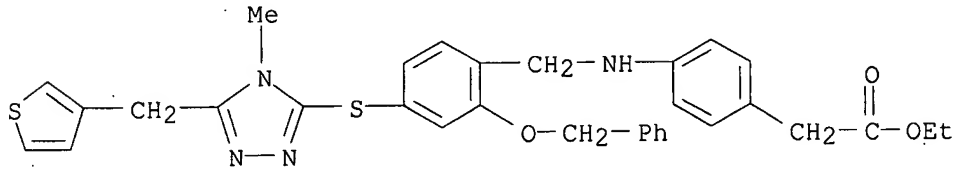
CN Benzeneacetic acid, 4-[[[4-[[4-methyl-5-(3-thienylmethyl)-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

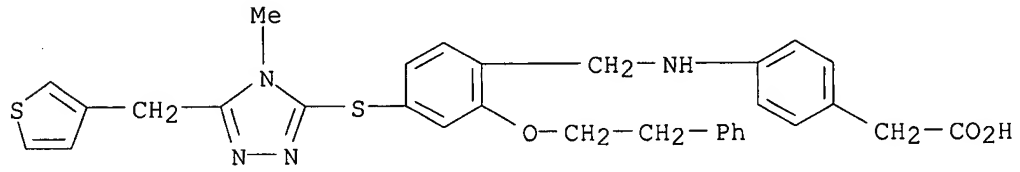
Updated Search



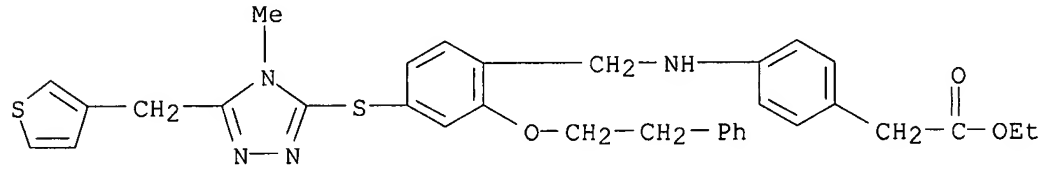
RN 854028-82-3 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-methyl-5-(3-thienylmethyl)-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 854028-83-4 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-methyl-5-(3-thienylmethyl)-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

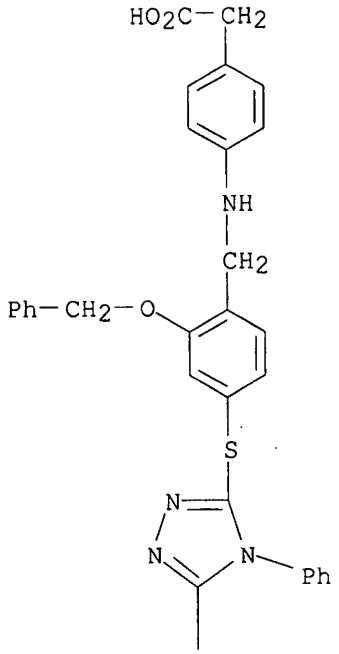


RN 854028-84-5 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[4-methyl-5-(3-thienylmethyl)-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 854028-89-0 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[[(2,3-dihydro-7-methyl-1H-inden-4-yl)oxy]methyl]-4-phenyl-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-A



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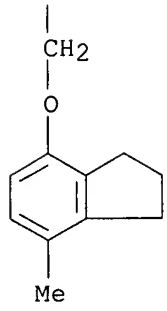
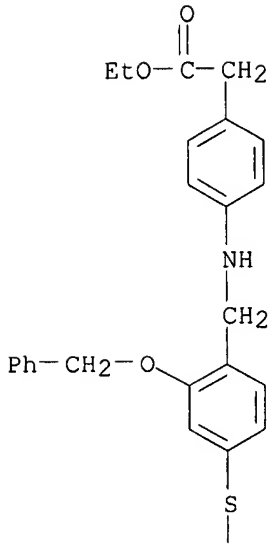


RN 854028-90-3 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[[(2,3-dihydro-7-methyl-1H-inden-4-yl)oxy]methyl]-4-phenyl-4H-1,2,4-triazol-3-yl]thio]-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

Updated Search

PAGE 1-A



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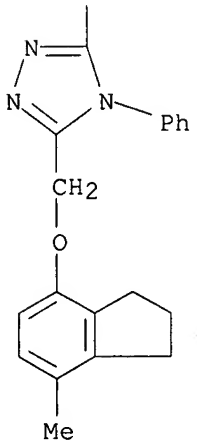

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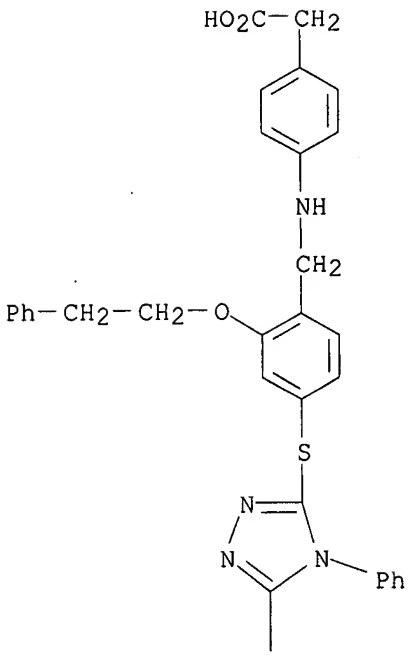
CN Benzeneacetic acid, 4-[[[4-[[5-[[(2,3-dihydro-7-methyl-1H-inden-4-yl)oxy]methyl]-4-phenyl-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Updated Search

PAGE 1-A



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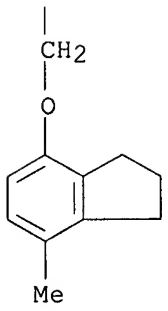
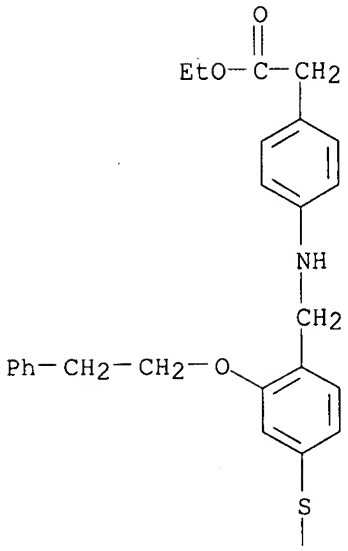


RN 854028-92-5 HCAPLUS
CN Benzeneacetic acid, 4-[[[4-[[5-[[(2,3-dihydro-7-methyl-1H-inden-4-yl)oxy]methyl]-4-phenyl-4H-1,2,4-triazol-3-yl]thio]-2-(2-phenylethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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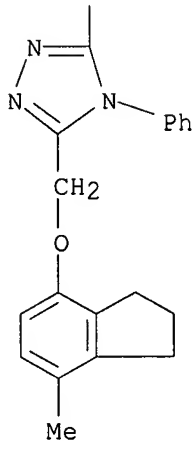


REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:456733 HCAPLUS
DOCUMENT NUMBER: 144:311763
TITLE: Synthesis and anti-inflammatory and analgesic activities of the derivatives of ibuprofen
AUTHOR(S): Guo, Chang-Bin; Chen, Xiao-Hong; Yi, Xiang; Guo, Zong-Ru; Chu, Feng-Ming; Cheng, Gui-Fang

Updated Search

10572578

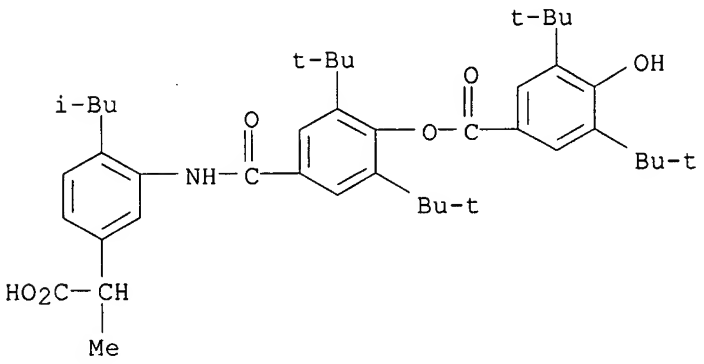
CORPORATE SOURCE: Institute of Material Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Huaxue Xuebao (2005), 63(9), 841-848
CODEN: HHHPA4; ISSN: 0567-7351
PUBLISHER: Kexue Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 144:311763

AB Based on the structural differences between cyclooxygenase-2 (COX-2) and COX-1, a series of ibuprofen derivs. was designed, in which, a substituted benzamido group was introduced to the 3 position of the Ph ring of ibuprofen. The purpose of this modification was to add a structural segment to occupy the side pocket in COX-2 so as to enhance their affinity for COX-2. Twelve target compds. were synthesized in five steps with ibuprofen as the starting material and structurally confirmed by 1H NMR, MS, and elemental anal. (or HRMS). The biol. tests showed that some of them have inhibitory activity against COX-2 in vitro. Compds. 7g and 7h were evaluated in vivo and exhibited weak anti-inflammatory but potent analgesic activities.

IT 879407-71-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and anti-inflammatory and analgesic activities of the derivs. of ibuprofen)

RN 879407-71-3 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxybenzoyl]oxy]-3,5-bis(1,1-dimethylethyl)benzoyl]amino]-α-methyl-4-(2-methylpropyl)- (9CI) (CA INDEX NAME)



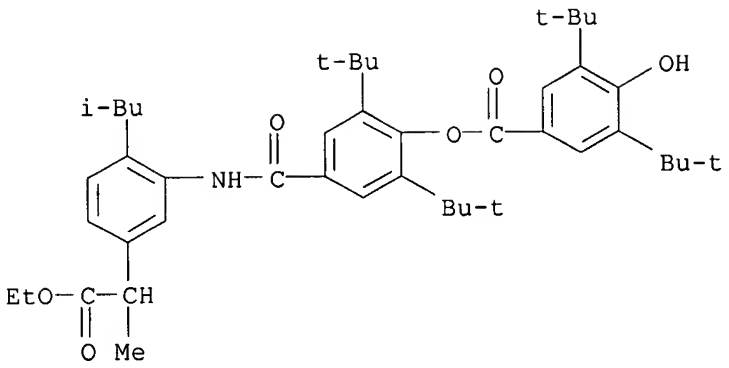
IT 879407-43-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and anti-inflammatory and analgesic activities of the derivs. of ibuprofen)

RN 879407-43-9 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxybenzoyl]oxy]-3,5-bis(1,1-dimethylethyl)benzoyl]amino]-α-methyl-4-(2-methylpropyl)-, ethyl ester (9CI) (CA INDEX NAME)

Updated Search

10572578



L17 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:999670 HCAPLUS
DOCUMENT NUMBER: 141:420447
TITLE: Method of treating atherosclerosis, dyslipidemias and related conditions
INVENTOR(S): Cheng, Kang; Waters, M. Gerard; Metters, Kathleen M.; O'Neill, Gary
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 33 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004229844	A1	20041118	US 2004-844773	20040513
AU 2004240597	A1	20041202	AU 2004-240597	20040513
CA 2525772	A1	20041202	CA 2004-2525772	20040513
WO 2004103370	A1	20041202	WO 2004-US14980	20040513
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1624871	A1	20060215	EP 2004-785539	20040513
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
BR 2004010273	A	20060516	BR 2004-10273	20040513
CN 1787819	A	20060614	CN 2004-80012853	20040513
JP 2006526030	T	20061116	JP 2006-515355	20040513
NO 2005005957	A	20060214	NO 2005-5957	20051214
PRIORITY APPLN. INFO.:			US 2003-470665P	P 20030515
			WO 2004-US14980	W 20040513

AB A method of treating atherosclerosis is disclosed wherein nicotinic acid or another nicotinic acid receptor agonist is administered to the patient

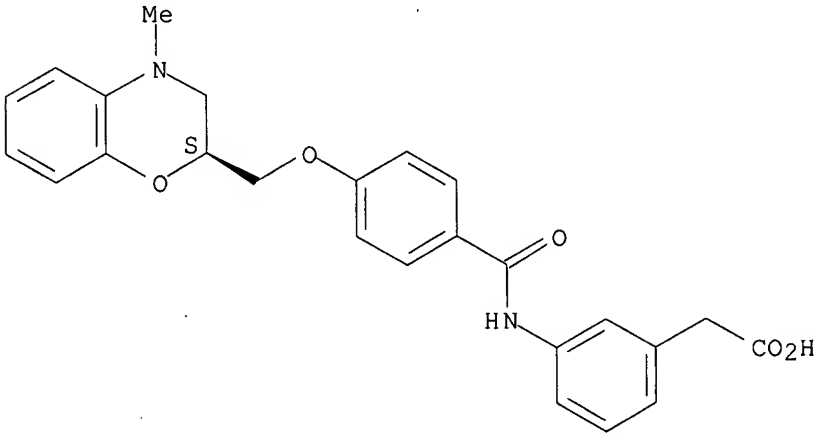
Updated Search

in combination with a DP receptor antagonist. The DP receptor antagonist is administered to reduce, prevent or eliminate flushing that may otherwise occur.

IT 603107-38-6P 794535-33-4P
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(method of treating atherosclerosis, dyslipidemias and related conditions)

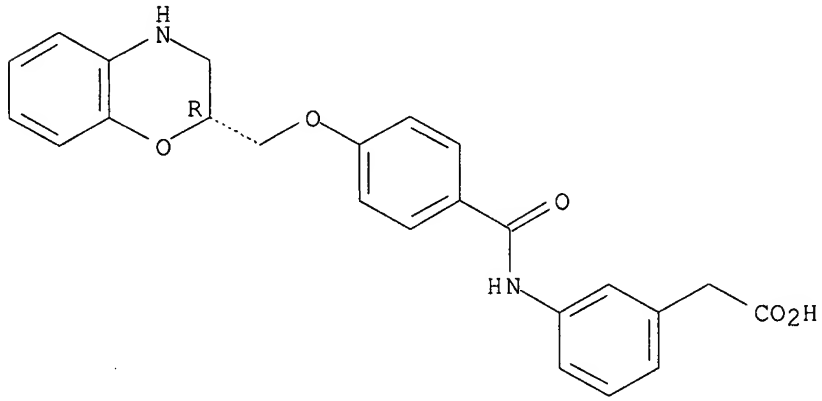
RN 603107-38-6 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 794535-33-4 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2R)-3,4-dihydro-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:931365 HCAPLUS

Updated Search

10572578

DOCUMENT NUMBER: 140:5078
TITLE: Preparation of dipyridodiazepine non-nucleoside reverse transcriptase inhibitors
INVENTOR(S): Simoneau, Bruno; Landry, Serge; Malenfant, Eric; Naud, Julie; O'meara, Jeffrey; Thavonekham, Bounkham; Yoakim, Christiane
PATENT ASSIGNEE(S): Boehringer Ingelheim International Gmbh, Germany
SOURCE: PCT Int. Appl., 79 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003097644	A2	20031127	WO 2003-CA718		20030514
WO 2003097644	A3	20040205			
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EP 1506195	A2	20050216	EP 2003-724719		20030514
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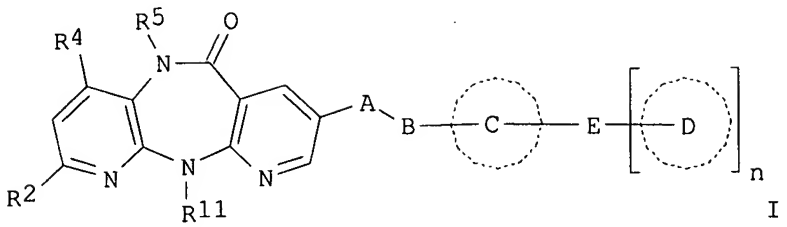
IN 2004DN02580	A	20070112	IN 2004-DN2580		20040902
NO 2004004104	A	20041201	NO 2004-4104		20040927
PRIORITY APPLN. INFO.:			US 2002-380886P	P	20020516
			WO 2003-CA718	W	20030514

OTHER SOURCE(S): MARPAT 140:5078
GI

Updated Search



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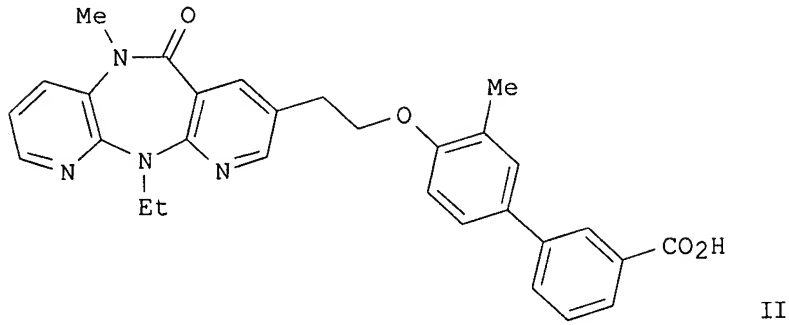


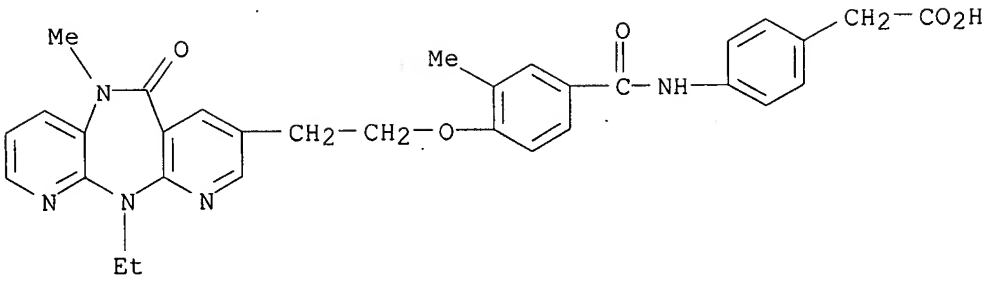
II

AB The title compds. [I; R2 = H, alkyl, halo, haloalkyl, OH, alkoxy, NH(alkyl) or N(alkyl)2; R4 = H, Me; R5 = H, Me; R11 = H, alkyl, cycloalkyl and alkylcycloalkyl; A = alkylene; B = O, S; n = 0-1; when n = 0, Ring C = (un)substituted 6-10 membered aryl, 5-6 membered heterocycle having from 1-4 heteroatoms selected from O, N, and S; E = CONR12R13 (R12, R13 = H, SO2alkyl, alkylCO2H, alkylcycloalkyl), CONHNR14R15 (R14, R15 = H, alkyl optionally substituted by CO2H), NR16COR17 (R16 = H, alkyl optionally substituted with CO2H, arylCO2H; R17 = alkenylCO2H, cycloalkylCO2H, NHalkylCO2H, etc.), NR18SO2alkyl (R18 = H, alkyl), SO2NR19R20 (R19 = H, alkyl; R20 = alkyl optionally substituted with CO2H), SO2R21 (R21 = alkyl); or when n = 1, Ring C is as defined above and E = a single bond or a connecting group; Ring D = (un)substituted 6-10 membered aryl, 5-6 membered heterocycle having from 1-4 heteroatoms selected from O, N, and S] or a salts or a prodrugs thereof, useful as inhibitors of HIV reverse transcriptase, were prepared Thus, reacting 11-ethyl-5,11-dihydro-8-(2-hydroxyethyl)-5-methyl-6H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one with Me 4'-hydroxy-3'-methyl-[1,1'-biphenyl]-4-carboxylate (preparation given) in the presence of DEAD, PPh3 in THF followed by hydrolysis of the resulting ester afforded II which showed IC50 of <10 nM in wild type RT assay. Pharmaceutical composition for the treatment or prevention of HIV infection, comprising the compound I is claimed.

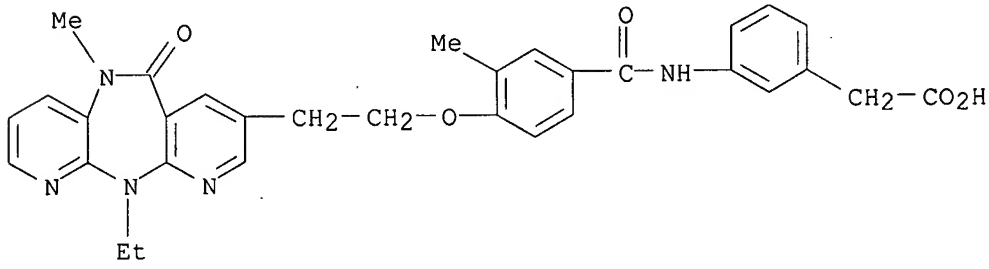
IT 627905-96-8P 627906-01-8P 627906-09-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dipyridodiazepine non-nucleoside reverse transcriptase inhibitors)

RN 627905-96-8 HCAPLUS

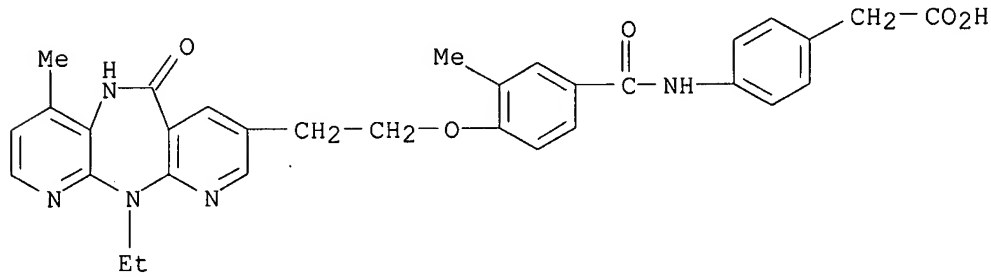
CN Benzeneacetic acid, 4-[[4-[2-(11-ethyl-6,11-dihydro-5-methyl-6-oxo-5H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-8-yl)ethoxy]-3-methylbenzoyl]amino]- (9CI) (CA INDEX NAME)



RN 627906-01-8 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[2-(11-ethyl-6,11-dihydro-5-methyl-6-oxo-5H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-8-yl)ethoxy]-3-methylbenzoyl]amino]- (9CI) (CA INDEX NAME)



RN 627906-09-6 HCAPLUS
CN Benzeneacetic acid, 4-[[4-[2-(11-ethyl-6,11-dihydro-4-methyl-6-oxo-5H-dipyrido[3,2-b:2',3'-e][1,4]diazepin-8-yl)ethoxy]-3-methylbenzoyl]amino]- (9CI) (CA INDEX NAME)



L17 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:154243 HCAPLUS
DOCUMENT NUMBER: 138:204839
TITLE: Preparation of benzamides affecting glucokinase for combined treatment or prevention of type 2 diabetes and obesity
INVENTOR(S): Boyd, Scott; Caulkett, Peter William Rodney; Hargreaves, Rodney Brian; Bowker, Suzanne Saxon; James, Roger; Johnstone, Craig; Jones, Clifford David; McKerrecher, Darren; Block, Michael Howard
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited

Updated Search

10572578

SOURCE: PCT Int. Appl., 156 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003015774	A1	20030227	WO 2002-GB3745	20020815
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2457410	A1	20030227	CA 2002-2457410	20020815
EP 1420784	A1	20040526	EP 2002-755165	20020815
EP 1420784	B1	20060419		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002012008	A	20040928	BR 2002-12008	20020815
HU 200401213	A2	20041228	HU 2004-1213	20020815
CN 1568185	A	20050119	CN 2002-820347	20020815
US 2005080106	A1	20050414	US 2003-486496	20020815
EP 1529530	A1	20050511	EP 2004-28298	20020815
EP 1529530	B1	20060802		
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NZ 531193	A	20050729	NZ 2002-531193	20020815
JP 2005525291	T	20050825	JP 2003-520733	20020815
EP 1568367	A1	20050831	EP 2004-28297	20020815
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AT 323487	T	20060515	AT 2002-755165	20020815
EP 1661567	A1	20060531	EP 2006-1805	20020815
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EP 1661568	A1	20060531	EP 2006-1806	20020815
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
EP 1661569	A1	20060531	EP 2006-1807	20020815
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EP 1661563	A1	20060531	EP 2006-1808	20020815
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EP 1669068	A1	20060614	EP 2006-1809	20020815
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EP 1669069	A1	20060614	EP 2006-1810	20020815
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
EP 1674097	A1	20060628	EP 2006-1796	20020815
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IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK					
AT 334678	T	20060815	AT 2004-28298		20020815
EP 1695705	A1	20060830	EP 2006-9486		20020815
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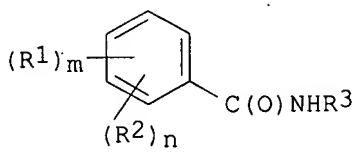
ZA 2004001015	A	20050506	ZA 2004-1015		20040206
IN 2004MN00118	A	20060203	IN 2004-MN118		20040216
NO 2004000686	A	20040217	NO 2004-686		20040217
HK 1064598	A1	20060929	HK 2004-107483		20040928
HK 1076042	A1	20070112	HK 2005-108225		20040928
JP 2005320343	A	20051117	JP 2005-168987		20050609
PRIORITY APPLN. INFO.:			SE 2001-2764	A	20010817
			EP 2002-755165	A3	20020815
			EP 2004-28298	A3	20020815
			JP 2003-520733	A3	20020815
			WO 2002-GB3745	W	20020815
			HK 2004-107483	A	20040928

OTHER SOURCE(S): MARPAT 138:204839

GI



I

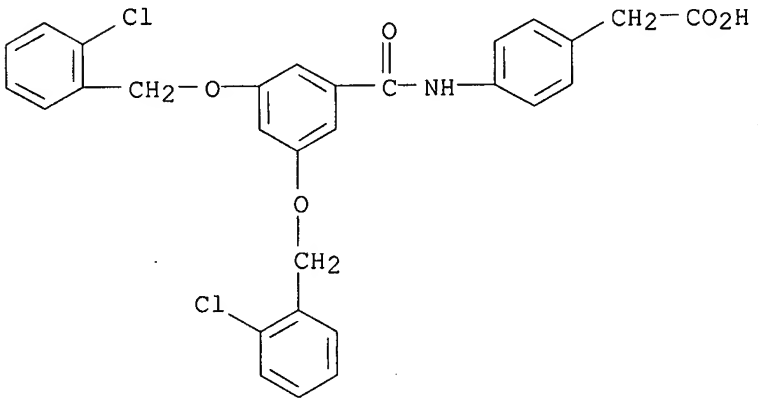
AB The invention relates to the use of benzamides (shown as I; variables defined below; e.g. 2-[[3,5-di(2-chlorobenzyloxy)benzoyl]amino]thiazole) or a salt, solvate or prodrug thereof, in the preparation of a medicament for the treatment or prevention of a disease condition mediated through glucokinase (GLK; no data), such as type 2 diabetes, and to the compds. I and methods for preparing them. Twelve pharmaceutical compns. are included. For I: m is 0-2; n is 0-4; and n + m > 0; each R1 = OH, -(CH2)1-4OH, -CH3-aFa, -(CH2)1-44CH3-aFa, -OCH3-aFa, halo, C1-6alkyl, C2-6alkenyl, C2-6alkynyl, NH2, -NH-C1-4alkyl, -N-di(C1-4alkyl), CN, formyl, Ph or heterocyclyl optionally substituted by C1-6alkyl. Each R2 is the group Y-X- wherein each X is a linker = -O-Z-, -O-Z-O-Z-, -C(O)O-Z-, -OC(O)-Z-, -S-Z-, -SO-Z-, -SO2-Z-, -N(R6)-Z-, -N(R6)SO2-Z-, -SO2N(R6)-Z-, -(CH2)1-4-, -CH:CH-Z-, -C.tplbond.C-Z-, -N(R6)CO-Z-, -CON(R6)-Z-, -C(O)N(R6)S(O)2-Z-, -S(O)2N(R6)C(O)-Z-, -C(O)-Z-, -Z-, -C(O)-Z-O-Z-, -N(R6)-C(O)-Z-O-Z-, -O-Z-N(R6)-Z-, -O-C(O)-Z-O-Z- or a direct bond; each Z = a direct bond, C2-6alkenylene or -(CH2)p-C(R6a)2-(CH2)q-; each Y = aryl-Z1-, heterocyclyl-Z1-, C3-7cycloalkyl-Z1-, C1-6alkyl, C2-6alkenyl, C2-6alkynyl, -(CH2)1-4CH3-aFa or -CH(OH)CH3-aFa; R3 = Ph or a heterocyclyl; addnl. details are given in the claims. More than 30 example prepns. of I are included and >300 specific examples of I are included with characterization data. For example, to prepare 2-[[3,5-di(2-chlorobenzyloxy)benzoyl]amino]thiazole, diisopropylethylamine (2.0 mmol) then 4-dimethylaminopyridine (0.1 mmol) were added to a solution of 2-aminothiazole (1.0 mmol) and 3,5-di(2-chlorobenzyloxy)benzoic acid chloride (1.0 mmol) in CH2Cl2 (10 mL) under Ar at ambient temperature After 80 mins the reaction mixture was filtered, washed with CH2Cl2 and dried under high vacuum to give the title compound as a colorless solid (41%).

IT 499991-42-3P, N-(4-(Carboxymethyl)phenyl)-3-((2-chlorophenyl)methoxy)-5-((2-chlorophenyl)methoxy)benzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

Updated Search

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzamides affecting glucokinase for combined treatment or prevention of type 2 diabetes and obesity)

RN 499991-42-3 HCAPLUS
CN Benzeneacetic acid, 4-[[3,5-bis[(2-chlorophenyl)methoxy]benzoyl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 13 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:367337 HCAPLUS
DOCUMENT NUMBER: 125:33683
TITLE: Aromatic amino ethers as pain relieving agents
INVENTOR(S): Breault, Gloria Anne; Oldfield, John; Tucker, Howard; Warner, Peter
PATENT ASSIGNEE(S): Zeneca Limited, UK
SOURCE: PCT Int. Appl., 140 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

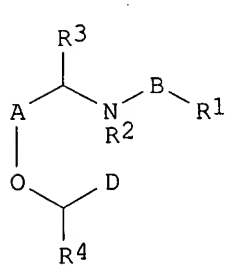
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9603380	A1	19960208	WO 1995-GB1728	19950721
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT, UA				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2192088	A1	19960208	CA 1995-2192088	19950721
AU 9529883	A	19960222	AU 1995-29883	19950721
AU 688541	B2	19980312		
EP 773930	A1	19970521	EP 1995-925943	19950721
EP 773930	B1	20001011		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1154106	A	19970709	CN 1995-194340	19950721

Updated Search

CN 1085663	B	20020529			
BR 9508335	A	19970930	BR 1995-8335		19950721
HU 76606	A2	19971028	HU 1996-3338		19950721
JP 10503487	T	19980331	JP 1995-505573		19950721
AT 196898	T	20001015	AT 1995-925943		19950721
ES 2150577	T3	20001201	ES 1995-925943		19950721
PT 773930	T	20010131	PT 1995-925943		19950721
TW 411328	B	20001111	TW 1995-84107606		19950722
ZA 9506149	A	19960207	ZA 1995-6149		19950724
FI 9700261	A	19970122	FI 1997-261		19970122
FI 116219	B1	20051014			
NO 9700314	A	19970313	NO 1997-314		19970124
NO 308032	B1	20000710			
US 5843942	A	19981201	US 1997-776275		19970124
CN 1286254	A	20010307	CN 2000-104017		20000310
GR 3034603	T3	20010131	GR 2000-402119		20001012
PRIORITY APPLN. INFO.:			GB 1994-14924	A	19940725
			GB 1995-1288	A	19950124
			WO 1995-GB1728	W	19950721

OTHER SOURCE(S): MARPAT 125:33683

GI



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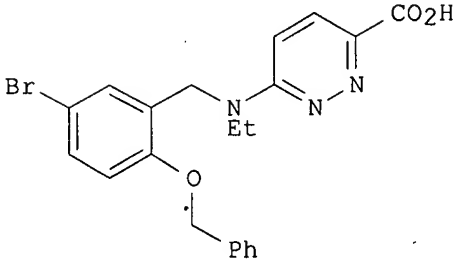


II

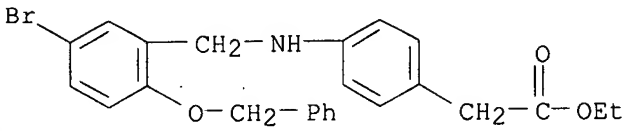
AB The invention relates to compds. I [A = (un)substituted Ph, naphthyl, pyridyl, pyrazinyl, pyridazinyl, pyrimidyl, thienyl, thiazolyl, oxazolyl, thiadiazolyl having ≥ 2 adjacent ring C atoms, or bicyclic ring system, provided that the shown sidechains on A are in a 1,2-relationship, and the 3-position is unsubstituted; B, D = (un)substituted ring system; R1 = various groups; R2 = H, alk(en/yn)yl, phenylalkyl, 5- or 6-membered heteroarylalkyl; R3, R4 = H or alkyl] and their N-oxides, S-oxides, pharmaceutically acceptable salts, and in vivo-hydrolyzable esters and amides. Also claimed are processes for their preparation, intermediates, use as therapeutic agents, and pharmaceutical compns. I are analgesics which are structurally different from NSAIDS and opiates, and which may also possess antiinflammatory, antipyretic, and antidiarrheal properties. For example, condensation of 6-chloropyridazine-3-carboxamide with N-ethyl-N-(2-benzyloxy-5-bromobenzyl)amine-HCl in N-methylpyrrolidinone containing NaHCO3 at 115° (85%), and hydrolysis of the carboxamide function with NaOH in iso-PrOH (97%), gave title compound II. I generally had pA2 > 5.3 for inhibition of PGE2-induced contraction of guinea pig ileum in vitro, and ED50 of 0.01-100 mg/kg orally in the i.p.-induced writhing test.

IT 177759-74-9P 177759-75-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of aromatic amino ethers as analgesics)

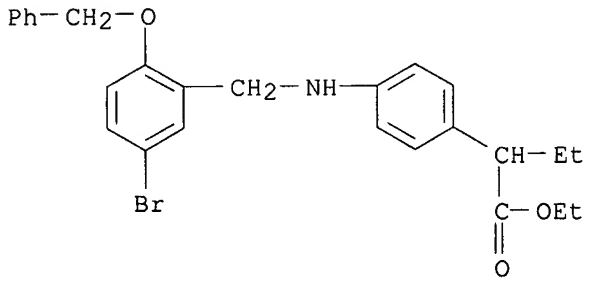
RN 177759-74-9 HCAPLUS

Updated Search

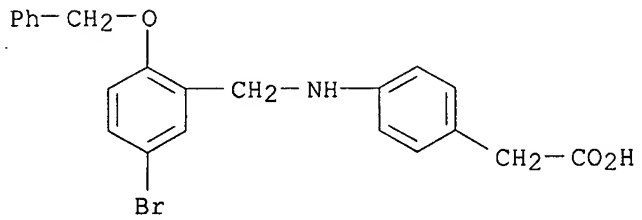
CN Benzeneacetic acid, 4-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 177759-75-0 HCAPLUS
CN Benzeneacetic acid, 4-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]amino]-α-ethyl-, ethyl ester (9CI) (CA INDEX NAME)



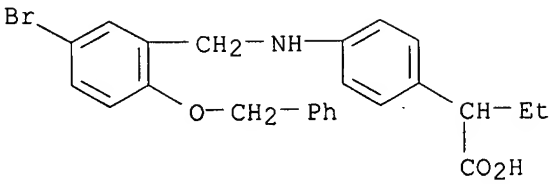
IT 177757-24-3P 177757-25-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aromatic amino ethers as analgesics)
RN 177757-24-3 HCAPLUS
CN Benzeneacetic acid, 4-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)



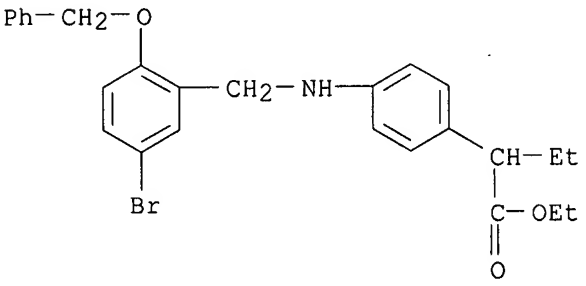
RN 177757-25-4 HCAPLUS
CN Benzeneacetic acid, 4-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]amino]-α-ethyl- (9CI) (CA INDEX NAME)

Updated Search

10572578



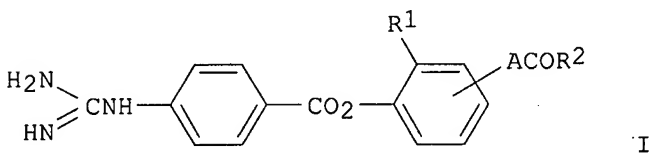
IT 177759-75-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of aromatic amino ethers as analgesics)
RN 177759-75-0 HCAPLUS
CN Benzeneacetic acid, 4-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]amino]-α-ethyl-, ethyl ester (9CI) (CA INDEX NAME)



L17 ANSWER 14 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:262466 HCAPLUS
DOCUMENT NUMBER: 124:342873
TITLE: Preparation of guanidinobenzoate esters as serine protease inhibitors
INVENTOR(S): Hashiguchi, Teruji; Inoe, Toshitaka; Ikesue, Koichi; Fujimoto, Noryuki; Takeda, Kazuhisa
PATENT ASSIGNEE(S): Hisamitsu Pharmaceutical Co, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08048664	A	19960220	JP 1994-204558	19940805

PRIORITY APPLN. INFO.: JP 1994-204558 19940805
OTHER SOURCE(S): MARPAT 124:342873
GI



I

Updated Search

AB Serine protease-inhibiting guanidinobenzoate esters I [A = (CH2)l, styryl; R1 = H, halo, lower alkyl; R2 = (CH2)mCOR3, (CH2)mCO2R4, NH(CH2)nCOR3, NH(CH2)nCO2R4, NHCHR5CO2R4, NHC6H4(CH2)pCO2R4; R3 = 2-thiazolylamino, (4,5-dimethylthiazol-2-yl)amino, 3,5-dichloroanilino, 2-pyridylamino, (5-methylisoxazol-3-yl)amino, piperidino, 2-methoxycarbonylanilino; R4 = H, lower alkyl, (un)substituted benzyl; R5 = (un)substituted benzyl, MeO2CCH2; l = 0-5; m = 2, 3; n = 1-5; p = 0, 1], useful for treatment of inflammation, allergy, pain, bleeding, thrombosis, etc., are prepared 4-Guanidinobenzoic acid hydrochloride (1.04 g) was treated with DCC in pyridine-DMF mixture at -15° for 20 min, treated with 1.33 g N-(2-thiazolyl)-3-(4-hydroxybenzoyl)propanamide at 0° overnight to give the corresponding ester. The ester was converted into 0.35 g dimethanesulfonate salt, which had IC50 of 0.0091 μM against kallikrein.

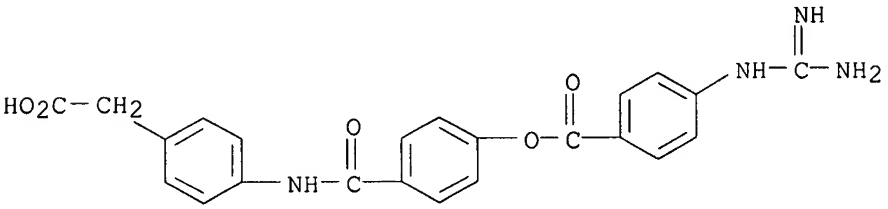
IT 176532-37-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of protease inhibitors from guanidinobenzoate and phenols for treatment of diseases)

RN 176532-37-9 HCAPLUS

CN Benzeneacetic acid, 4-[[4-[[4-[(aminoiminomethyl)amino]benzoyl]oxy]benzoyl]amino]-, monomethanesulfonate (9CI) (CA INDEX NAME)

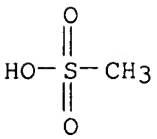
CM 1

CRN 176532-36-8
CMF C23 H20 N4 O5



CM 2

CRN 75-75-2
CMF C H4 O3 S



L17 ANSWER 15 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:7392 HCAPLUS
DOCUMENT NUMBER: 112:7392
TITLE: Preparation of quinoline derivatives as lipoxygenase

Updated Search

10572578

inhibitors and leukotriene antagonists

INVENTOR(S): Ahnfelt-Roenne, Ian; Torngaard Hansen, Erik; Kirstein, Dorte; Tvaermose Nielsen, Ole Bent; Rachlin, Schneur

PATENT ASSIGNEE(S): Leo Pharmaceutical Products Ltd., Den.

SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2

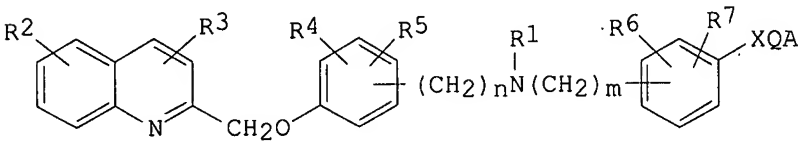
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8905294	A1	19890615	WO 1988-DK188	19881117
W: AU, DK, JP, KR, US				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AU 8826118	A	19890705	AU 1988-26118	19881117
AU 617386	B2	19911128		
JP 03501477	T	19910404	JP 1989-500028	19881117
EP 420844	A1	19910410	EP 1989-900021	19881117
EP 420844	B1	19940824		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
ZA 8808763	A	19890726	ZA 1988-8763	19881123
CA 1336602	C	19950808	CA 1988-584360	19881128
ES 2011919	A6	19900216	ES 1988-3652	19881130
DK 9001183	A	19900514	DK 1990-1183	19900514
DK 170576	B1	19951030		
US 5110819	A	19920505	US 1990-476403	19900601

PRIORITY APPLN. INFO.: GB 1987-28051 A 19871201
WO 1988-DK188 A 19881117

OTHER SOURCE(S): MARPAT 112:7392

GI



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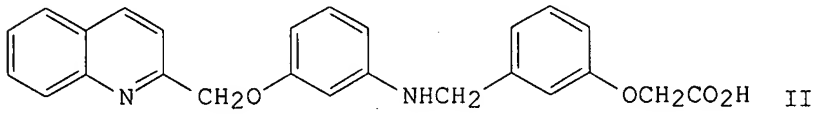


II

AB Quinolinylmethoxyanilines [I; R1, R8 = H, (un)saturated (un)substituted alkyl, aryl, aralkyl; R2-R7 = H, (pseudo)halo, cyano, NO2, CO2H, carbalkoxy, carbamyl, OH, alkoxy, alkyl, (un)substituted amino; n, m = 0-6; X = bond, O, S, S(O), S(O)2, NR8; Q = bond, alkylene; A = acidic group, e.g. CO2H, 1H-tetrazolyl, sulfamyl, or sulfonic/sulfinic/hydroxamic acid; n ≠ 0 when A = CO2H and X = Q = bond] and their salts and esters were prepared as lipoxygenase inhibitors and/orleukotriene antagonists. Thus, condensation of 3-(2-quinolylmethoxy)aniline with 3-OHCC6H4OCH2CO2Hin MeOH precipitated the corresponding imine, which was reduced by NaBH4 in EtOH to give (quinolylmethoxy)(carboxymethoxybenzyl)aniline II. In a test for leukotriene antagonism using guinea pig tracheal strips, the pKB for II was 8.3; pKB values of other prepared antagonists also correlated with

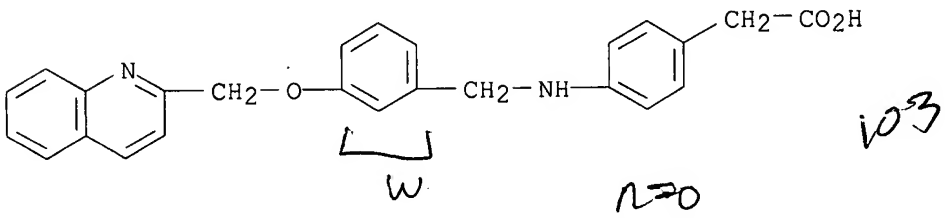
Updated Search

inhibition of LTD4 receptor binding.

IT 124038-67-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as lipoxygenase inhibitor and leukotriene antagonist)

RN 124038-67-1 HCAPLUS

CN Benzeneacetic acid, 4-[[[3-(2-quinolinylmethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)



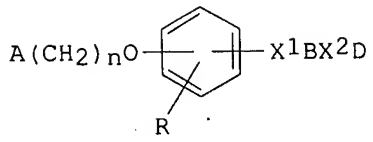
L17 ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:439428 HCAPLUS
DOCUMENT NUMBER: 107:39428
TITLE: Preparation of phenylene derivatives as allergy inhibitors
INVENTOR(S): Mase, Toshiyasu; Murase, Kiyoshi; Hara, Hiromu; Tomioka, Kenichi
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 210 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8605779	A1	19861009	WO 1986-JP155	19860331
W: JP, KR, US				
RW: AT, BE, CH, DE, FR, GB, IT, NL, SE				
EP 218728	A1	19870422	EP 1986-902035	19860331
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
JP 63159342	A	19880702	JP 1986-76958	19860403
CA 1273940	A1	19900911	CA 1986-505780	19860403
US 4994479	A	19910219	US 1986-899218	19860815
US 5116853	A	19920526	US 1989-413458	19890927
US 5140046	A	19920818	US 1990-567159	19900813
PRIORITY APPLN. INFO.:			JP 1985-70566 A	19850403
			JP 1985-297096 A	19851226
			WO 1986-JP155 W	19860331
			US 1986-899218 A3	19860815

GI

10572578



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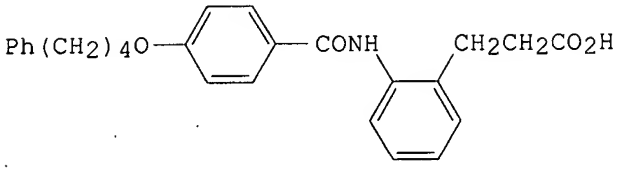


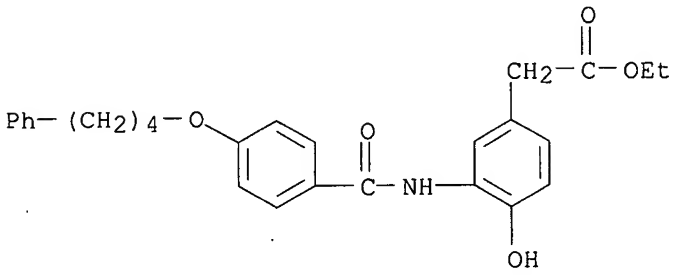
II

AB The title compds. [I; A = H, Ph, PhO; B = 1,3,4-thiadiazole-2,5-diyl, (un)substituted phenylene, indanylene; D = CO2H, alkoxycarbonyl, tetrazol-5-yl; R = H, alkoxy; X1 = CH2CH2, CH:CH, CH2Y1, Y1CH2, COY2, Y2CO; X2 = CH:CH, Y1Y3; Y1 = O, S, NH; Y2 = NH, CH2Y1, Y1CH2; Y3 = C1-6 alkylene, optionally interrupted by S] were prepared as inhibitors of SRS-A, useful in treating allergic diseases. p-Ph(CH2)4OC6H4CO2H was converted to its acid chloride and used to acylate 2-H2NC6H4CH2CH2CO2Et. The product was saponified to give (benzoylamino)benzyenepropanoic acid II. II inhibited the SRS-A-induced contraction of guinea pig ileum with an IC50 of 3.3 + 10-8M.

IT 108807-35-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-alkylation of)

RN 108807-35-8 HCAPLUS

CN Benzeneacetic acid, 4-hydroxy-3-[[4-(4-phenylbutoxy)benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



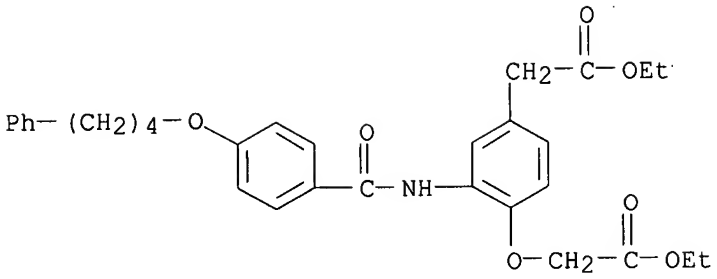
102

IT 108806-58-2P 108806-82-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as allergy inhibitor)

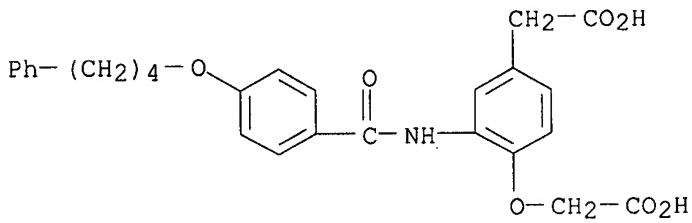
RN 108806-58-2 HCAPLUS

CN Benzeneacetic acid, 4-(2-ethoxy-2-oxoethoxy)-3-[[4-(4-phenylbutoxy)benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

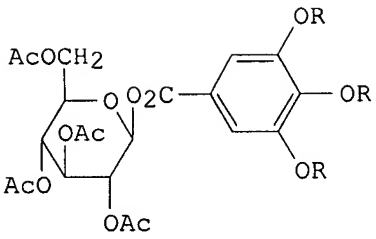
Updated Search



RN 108806-82-2 HCAPLUS
CN Benzeneacetic acid, 4-(carboxymethoxy)-3-[[4-(4-phenylbutoxy)benzoyl]amino]- (9CI) (CA INDEX NAME)



L17 ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1981:604308 HCAPLUS
DOCUMENT NUMBER: 95:204308
TITLE: Synthesis and study of derivatives of 2,3,4,6-tetraacetylglucose acylated with 3,4,5-(tribenzyloxy)-, 3,4,5-trihydroxy-, and 3,4,5-trimethoxybenzoic acids
AUTHOR(S): Dziuviene, D.; Didzepetriene, J.; Degutis, J.
CORPORATE SOURCE: Nauchno-Issled. Inst. Onkol., Vilnius, USSR
SOURCE: Zhurnal Obshchei Khimii (1981), 51(8), 1894-6
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



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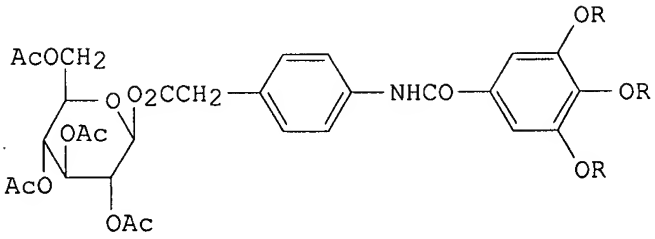


II

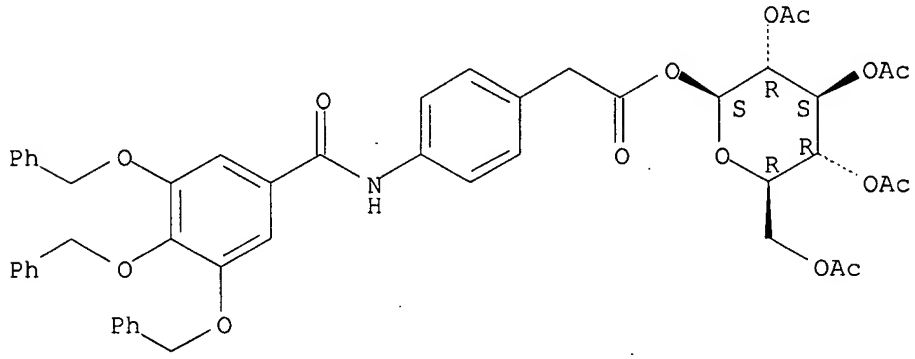
AB Glucopyranose benzoate I (R = PhCH2) was prepared in 94.8% yield by esterification of 2,3,4,6-tetra-O-acetyl-β-D-glucopyranose with 3,4,5-(RO)3C6H2COCl. Subsequent hydrogenolysis gave 80.8% I (R = H). Analogous treatment of 1-(p-aminophenylacetyl)-2,3,4,6-tetra-O-acetyl-β-D-glucopyranose gave 94.4% II (R = PhCH2) which was hydrogenolyzed to give 87.4% II (R = H). I and II (R = Me) were obtained by previously described methods. I and II are useful as neoplasm inhibitors.

IT 79814-55-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, hydrogenolysis, and neoplasm inhibiting activity of)

RN 79814-55-4 HCAPLUS

CN β-D-Glucopyranose, 2,3,4,6-tetraacetate 1-[4-[[3,4,5-tris(phenylmethoxy)benzoyl]amino]benzeneacetate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 18 OF 18 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:157682 HCAPLUS
DOCUMENT NUMBER: 92:157682
TITLE: Search for antileukotic and antineoplastic compounds among N-oxides of dimethylamino acids and derivatives

Updated Search

10572578

of trihydroxybenzoic acid

AUTHOR(S): Kutorga, V.; Didzepetriene, J.; Sukeliene, D.; Dziuviene, D.

CORPORATE SOURCE: Nauchno-Issled. Inst. Onkol., Vilnius, USSR

SOURCE: Sint. Izuch. Nov. Otechestvennykh Protivoleikoznykh Prep., Tezisy Konf. (1979), 67. Editor(s): Sadauskas, P. B. Akad. Nauk Litovskoi SSR, Inst. Biokhim.: Vilnius, USSR.
CODEN: 42MYAU

DOCUMENT TYPE: Conference

LANGUAGE: Russian

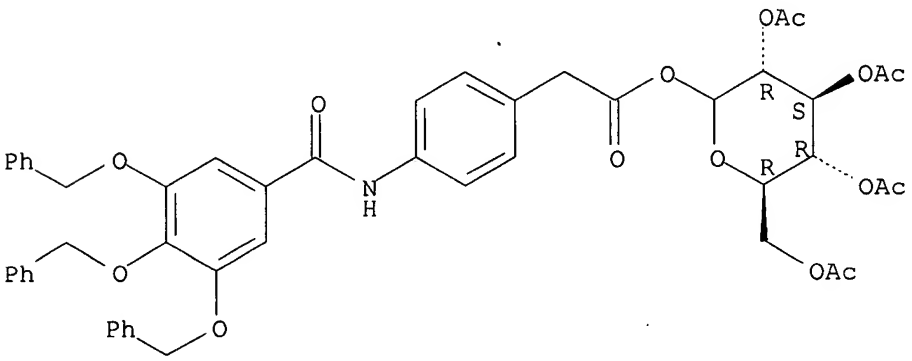
AB Of the 6 N-oxides of dimethylamino acids tested, dimethylglycine N-oxide Et ester [62227-32-1] appeared to be the most active, inhibiting L-1210 leukemia and the growth of solid tumors (sarcoma and carcinosarcoma) and prolonging the life span of animals with Ehrlich ascites tumors. Of the 6 trihydroxybenzoic acid derivs. tested, only 1-galloyl-2,3,4,6-tetraacetylglucose [73165-85-2] showed any antitumor activity.

IT 73165-86-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(neoplasm inhibition by)

RN 73165-86-3 HCAPLUS

CN D-Glucopyranose, 2,3,4,6-tetraacetate 1-[4-[[3,4,5-tris(phenylmethoxy)benzoyl]amino]benzeneacetate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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10572578

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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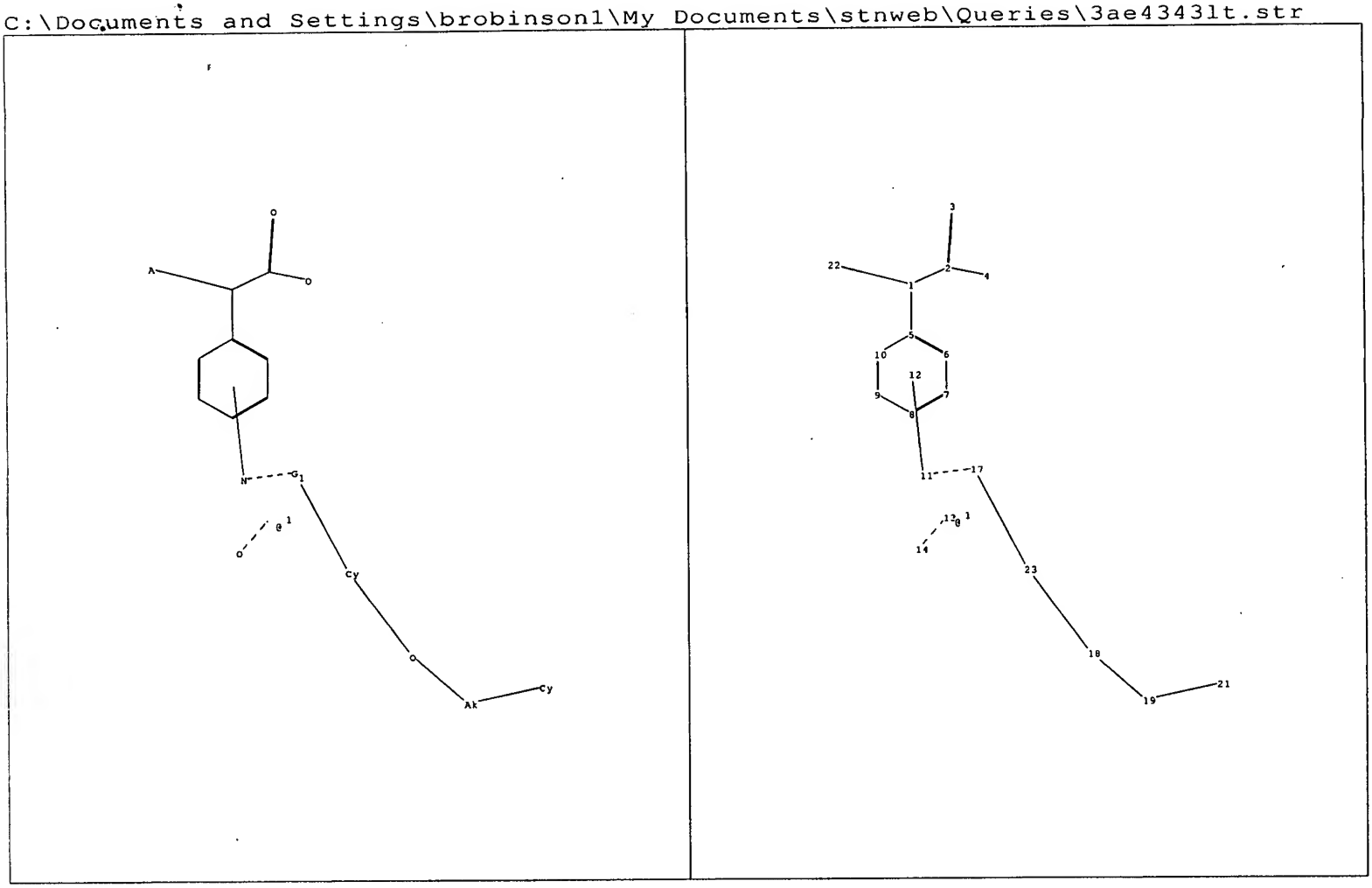

chain nodes :
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ring nodes :
5 6 7 8 9 10
chain bonds :
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ring bonds :
5-6 5-10 6-7 7-8 8-9 9-10
exact/norm bonds :
1-22 2-3 2-4 11-17 13-14 17-23 18-19 18-23 19-21
exact bonds :
1-2 1-5
normalized bonds :
5-6 5-10 6-7 7-8 8-9 9-10
isolated ring systems :
containing 1 : 5 :

G1:CH2,SO2,[*1]

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:CLASS 12:Atom 13:CLASS 14:CLASS 17:CLASS 18:CLASS
19:CLASS 21:CLASS 22:CLASS 23:Atom

10572578

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NEWS 4	DEC 18	CA/CAplus patent kind codes updated
NEWS 5	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 6	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS 7	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS 8	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS 9	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS 10	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS 11	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS 12	JAN 22	CA/CAplus updated with revised CAS roles
NEWS 13	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS 14	JAN 29	PHAR reloaded with new search and display fields
NEWS 15	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 16	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS 17	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS 18	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS 19	FEB 26	MEDLINE reloaded with enhancements
NEWS 20	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS 21	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS 22	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS 23	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS 24	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 25	MAR 16	CASREACT coverage extended
NEWS 26	MAR 20	MARPAT now updated daily
NEWS 27	MAR 22	LWPI reloaded
NEWS 28	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 29	MAR 30	INPADOCDB will replace INPADOC on STN
NEWS 30	APR 02	JICST-EPLUS removed from database clusters and STN

NEWS EXPRESS	NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

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10572578

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FULL ESTIMATED COST	0.21	0.21

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DICTIONARY FILE UPDATES: 5 APR 2007 HIGHEST RN 929247-80-3

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Updated Search

10572578

BATCH **COMPLETE**
PROJECTED ITERATIONS: 585280 TO 605920
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

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FULL SCREEN SEARCH COMPLETED - 597654 TO ITERATE

100.0% PROCESSED 597654 ITERATIONS 13 ANSWERS
SEARCH TIME: 00.00.06

L3 13 SEA SSS FUL L1

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FULL ESTIMATED COST 173.90 174.11

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FILE COVERS 1907 - 6 Apr 2007 VOL 146 ISS 16
FILE LAST UPDATED: 5 Apr 2007 (20070405/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3
L4 3 L3

=> d l4, ibib abs hitstr, 1-3

L4 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:456733 HCAPLUS
DOCUMENT NUMBER: 144:311763
TITLE: Synthesis and anti-inflammatory and analgesic activities of the derivatives of ibuprofen
AUTHOR(S): Guo, Chang-Bin; Chen, Xiao-Hong; Yi, Xiang; Guo, Zong-Ru; Chu, Feng-Ming; Cheng, Gui-Fang
CORPORATE SOURCE: Institute of Material Medica, Chinese Academy of

Updated Search

10572578

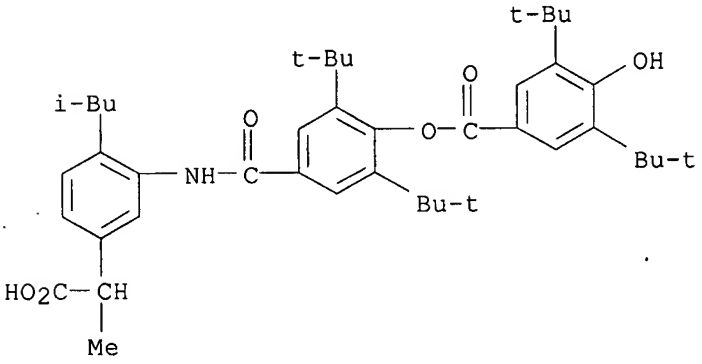
Medical Sciences and Peking Union Medical College, Beijing, 100050, Peop. Rep. China
SOURCE: Huaxue Xuebao (2005), 63(9), 841-848
CODEN: HHHPA4; ISSN: 0567-7351
PUBLISHER: Kexue Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 144:311763

AB Based on the structural differences between cyclooxygenase-2 (COX-2) and COX-1, a series of ibuprofen derivs. was designed, in which, a substituted benzamido group was introduced to the 3 position of the Ph ring of ibuprofen. The purpose of this modification was to add a structural segment to occupy the side pocket in COX-2 so as to enhance their affinity for COX-2. Twelve target compds. were synthesized in five steps with ibuprofen as the starting material and structurally confirmed by 1H NMR, MS, and elemental anal. (or HRMS). The biol. tests showed that some of them have inhibitory activity against COX-2 in vitro. Compds. 7g and 7h were evaluated in vivo and exhibited weak anti-inflammatory but potent analgesic activities.

IT 879407-71-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and anti-inflammatory and analgesic activities of the derivs. of ibuprofen)

RN 879407-71-3 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxybenzoyl]oxy]-3,5-bis(1,1-dimethylethyl)benzoyl]amino]-α-methyl-4-(2-methylpropyl)- (9CI) (CA INDEX NAME)



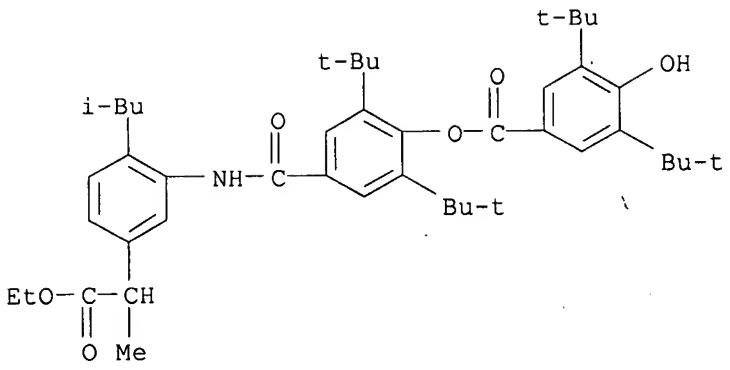
IT 879407-43-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and anti-inflammatory and analgesic activities of the derivs. of ibuprofen)

RN 879407-43-9 HCAPLUS

CN Benzeneacetic acid, 3-[[4-[[3,5-bis(1,1-dimethylethyl)-4-hydroxybenzoyl]oxy]-3,5-bis(1,1-dimethylethyl)benzoyl]amino]-α-methyl-4-(2-methylpropyl)-, ethyl ester (9CI) (CA INDEX NAME)

Updated Search

10572578



L4 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:281799 HCAPLUS
DOCUMENT NUMBER: 142:355273
TITLE: Preparation of benzoxazine compounds containing carboxylic acid moiety as DP receptor antagonists
INVENTOR(S): Naganawa, Atsushi; Iwahashi, Maki; Kinoshita, Atsushi; Shimabukuro, Atsushi; Ogawa, Seiji; Yano, Koji; Kobayashi, Kaoru; Okada, Yutaka; Kishida, Yoko; Kawauchi, Shouji; Tsukamoto, Kohki; Matsunaga, Yoko; Nambu, Fumio
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 151 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005028455	A1	20050331	WO 2004-JP13983		20040916
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2004274324	A1	20050331	AU 2004-274324		20040916
CA 2539070	A1	20050331	CA 2004-2539070		20040916
EP 1666473	A1	20060607	EP 2004-773373		20040916
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
BR 2004014487	A	20061114	BR 2004-14487		20040916
CN 1882554	A	20061220	CN 2004-80033868		20040916
NO 2006001207	A	20060619	NO 2006-1207		20060315
US 2007004716	A1	20070104	US 2006-572578		20060317
PRIORITY APPLN. INFO.:			JP 2003-325198	A	20030917
			JP 2004-101863	A	20040331

Updated Search

10572578

WO 2004-JP13983 W 20040916

OTHER SOURCE(S): MARPAT 142:355273
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = H, alkyl, etc.; R2 = halo, etc.; R3 = halo, etc.; R4 = H, alkyl, etc.; R5 = alkyl, etc.; R12, R13 = alkyl, etc.; W = mono- or bi-carbocyclic ring, etc.; G = alkylene having N, O, S, etc.; J = mono- or bicarbocyclic ring, mono- or biheterocyclic ring; m = 1-4; n = 0-4; i = 1-11; further details on m, n, i, R2, R3, R5 are given.] were prepared For example, acylation of 3-amino-4-fluorophenylacetic acid Me ester with compound II followed by hydrolysis using aqueous NaOH afforded compound III.

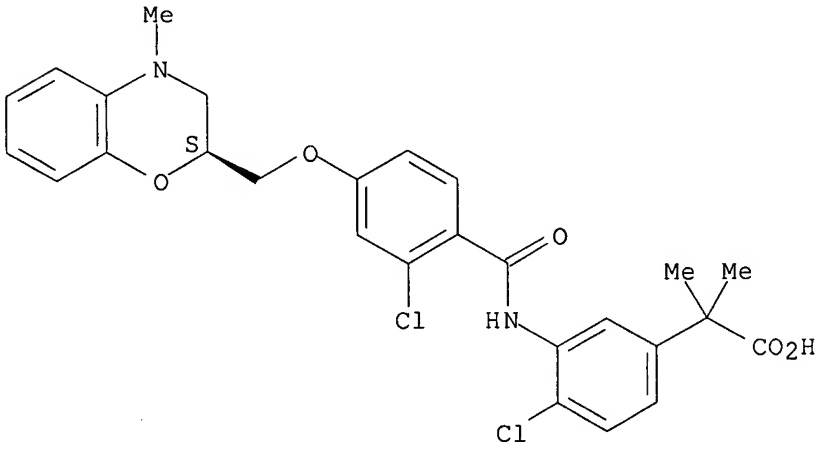
In DP (D prostanoid) receptor binding assays, compds. I exhibited the IC50 values of ≤10 μmol/L. Compds. I are claimed useful for the treatment of allergy, inflammation, etc. Formulations are given.

IT 848846-58-2P 848846-59-3P 848846-61-7P
848846-62-8P 848846-63-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoxazine compds. containing carboxylic acid moiety as DP receptor antagonists for treatment of allergy, inflammation, etc.)

RN 848846-58-2 HCAPLUS

CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α,α-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

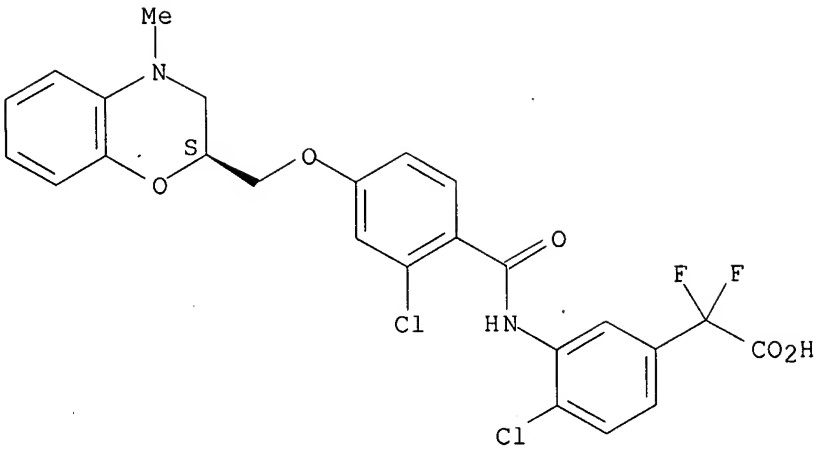


RN 848846-59-3 HCAPLUS

CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α,α-difluoro- (9CI) (CA INDEX NAME)

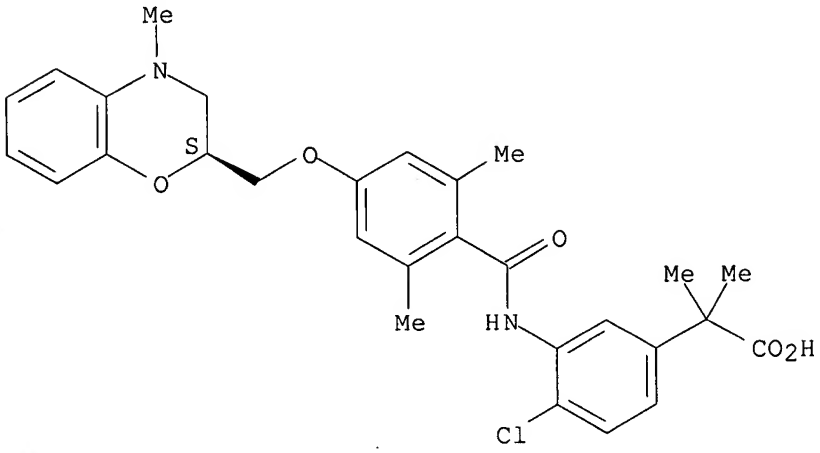
Absolute stereochemistry.

Updated Search



RN 848846-61-7 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,6-dimethylbenzoyl]amino]-α,α-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 848846-62-8 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]-α,α-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Updated Search

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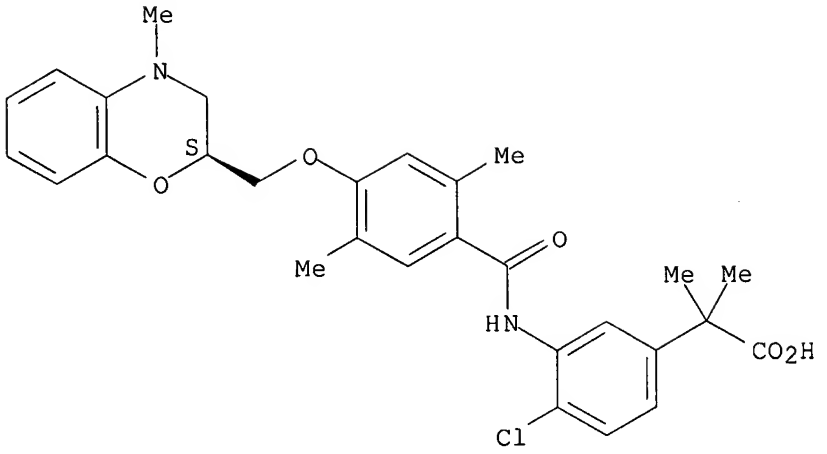
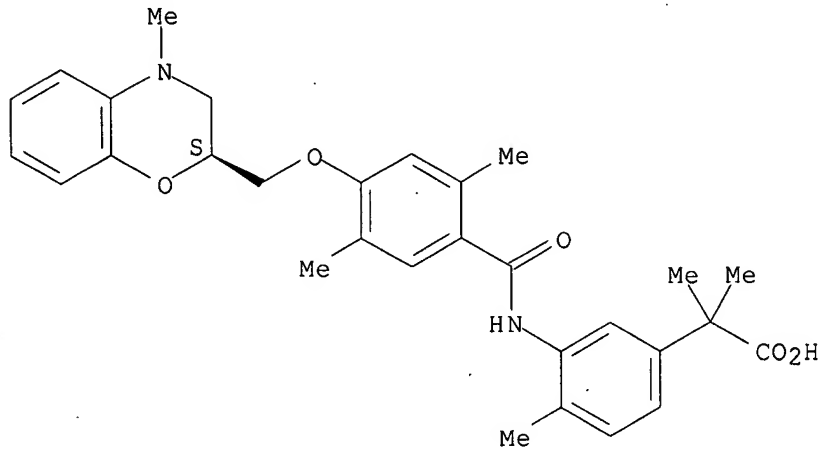


RN 848846-63-9 HCAPLUS
CN Benzeneacetic acid, 3-[[4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]-2,5-dimethylbenzoyl]amino]-α,α,4-trimethyl- (9CI) (CA INDEX NAME)

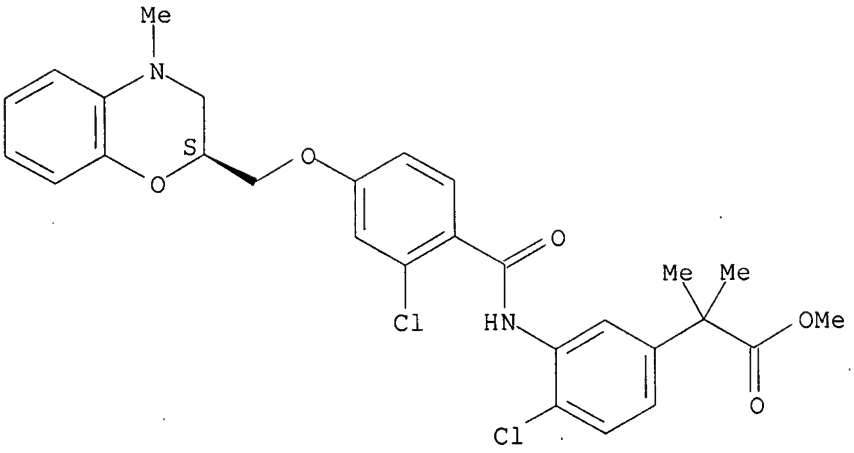
Absolute stereochemistry.



IT 848846-73-1P 848846-78-6P 848846-81-1P
848846-82-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzoxazine compds. containing carboxylic acid moiety as DP receptor antagonists for treatment of allergy, inflammation, etc.)
RN 848846-73-1 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α,α-dimethyl-, methyl ester (9CI) (CA INDEX NAME)

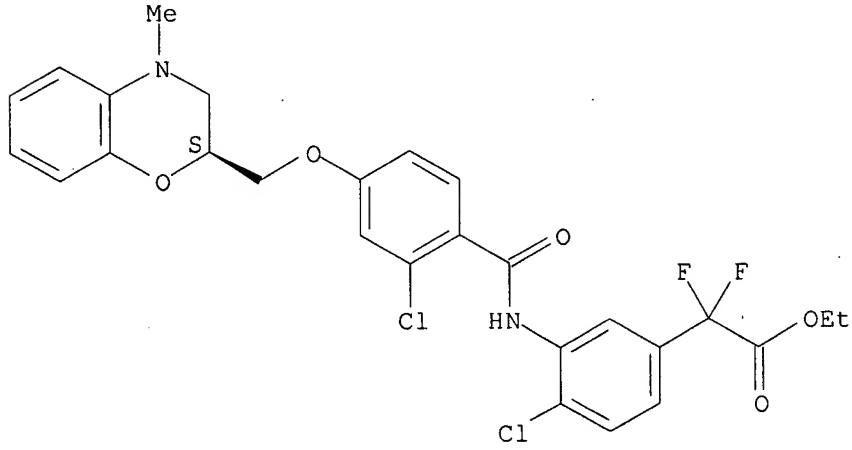
Absolute stereochemistry.

Updated Search



RN 848846-78-6 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α,α-difluoro-, ethyl ester (9CI) (CA INDEX NAME)

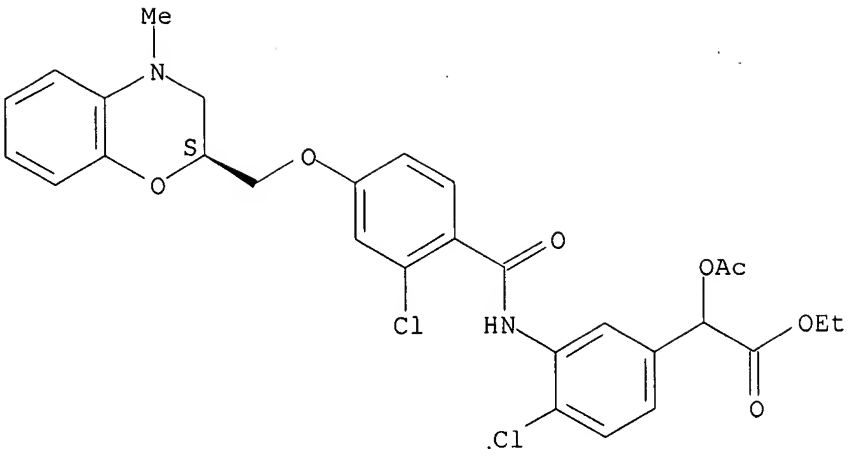
Absolute stereochemistry.



RN 848846-81-1 HCAPLUS
CN Benzeneacetic acid, α-(acetyloxy)-4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

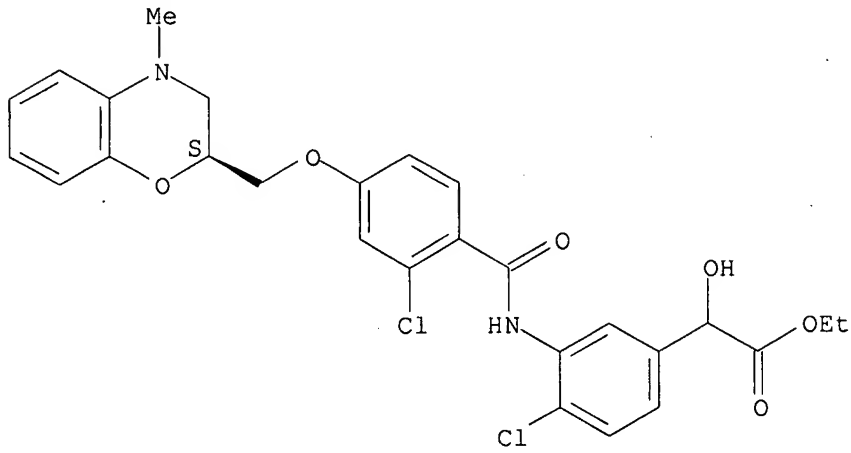
Absolute stereochemistry.

10572578



RN 848846-82-2 HCAPLUS
CN Benzeneacetic acid, 4-chloro-3-[[2-chloro-4-[[(2S)-3,4-dihydro-4-methyl-2H-1,4-benzoxazin-2-yl]methoxy]benzoyl]amino]-α-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:367337 HCAPLUS
DOCUMENT NUMBER: 125:33683
TITLE: Aromatic amino ethers as pain relieving agents
INVENTOR(S): Breault, Gloria Anne; Oldfield, John; Tucker, Howard; Warner, Peter
PATENT ASSIGNEE(S): Zeneca Limited, UK
SOURCE: PCT Int. Appl., 140 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Updated Search

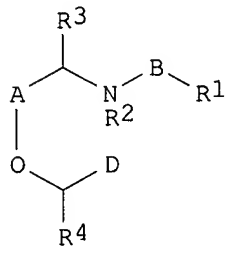
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9603380	A1	19960208	WO 1995-GB1728	19950721
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT, UA				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2192088	A1	19960208	CA 1995-2192088	19950721
AU 9529883	A	19960222	AU 1995-29883	19950721
AU 688541	B2	19980312		
EP 773930	A1	19970521	EP 1995-925943	19950721
EP 773930	B1	20001011		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1154106	A	19970709	CN 1995-194340	19950721
CN 1085663	B	20020529		
BR 9508335	A	19970930	BR 1995-8335	19950721
HU 76606	A2	19971028	HU 1996-3338	19950721
JP 10503487	T	19980331	JP 1995-505573	19950721
AT 196898	T	20001015	AT 1995-925943	19950721
ES 2150577	T3	20001201	ES 1995-925943	19950721
PT 773930	T	20010131	PT 1995-925943	19950721
TW 411328	B	20001111	TW 1995-84107606	19950722
ZA 9506149	A	19960207	ZA 1995-6149	19950724
FI 9700261	A	19970122	FI 1997-261	19970122
FI 116219	B1	20051014		
NO 9700314	A	19970313	NO 1997-314	19970124
NO 308032	B1	20000710		
US 5843942	A	19981201	US 1997-776275	19970124
CN 1286254	A	20010307	CN 2000-104017	20000310
GR 3034603	T3	20010131	GR 2000-402119	20001012

PRIORITY APPLN. INFO.:

GB 1994-14924	A	19940725
GB 1995-1288	A	19950124
WO 1995-GB1728	W	19950721

OTHER SOURCE(S): MARPAT 125:33683

GI



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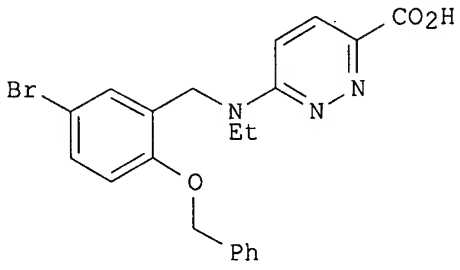

II

AB The invention relates to compds. I [A = (un)substituted Ph, naphthyl, pyridyl, pyrazinyl, pyridazinyl, pyrimidyl, thienyl, thiazolyl, oxazolyl, thiadiazolyl having ≥ 2 adjacent ring C atoms, or bicyclic ring system, provided that the shown sidechains on A are in a 1,2-relationship, and the 3-position is unsubstituted; B, D = (un)substituted ring system; R1 = various groups; R2 = H, alk(en/yn)yl, phenylalkyl, 5- or 6-membered

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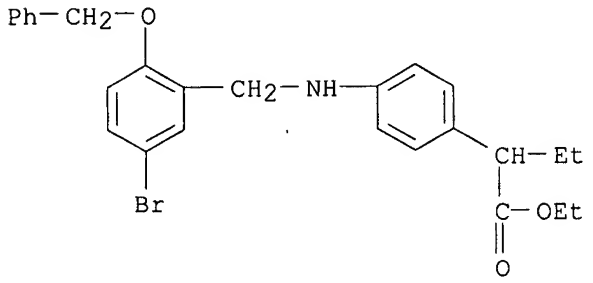
heteroarylalkyl; R3, R4 = H or alkyl] and their N-oxides, S-oxides, pharmaceutically acceptable salts, and in vivo-hydrolyzable esters and amides. Also claimed are processes for their preparation, intermediates, use as therapeutic agents, and pharmaceutical compns. I are analgesics which are structurally different from NSAIDS and opiates, and which may also possess antiinflammatory, antipyretic, and antidiarrheal properties. For example, condensation of 6-chloropyridazine-3-carboxamide with N-ethyl-N-(2-benzyloxy-5-bromobenzyl)amine-HCl in N-methylpyrrolidinone containing NaHCO3 at 115° (85%), and hydrolysis of the carboxamide function with NaOH in iso-PrOH (97%), gave title compound II. I generally had pA2 > 5.3 for inhibition of PGE2-induced contraction of guinea pig ileum in vitro, and ED50 of 0.01-100 mg/kg orally in the i.p.-induced writhing test.

IT 177759-75-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of aromatic amino ethers as analgesics)

RN 177759-75-0 HCAPLUS

CN Benzeneacetic acid, 4-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]amino]-α-ethyl-, ethyl ester (9CI) (CA INDEX NAME)

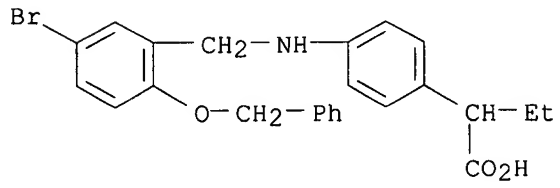


A

IT 177757-25-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aromatic amino ethers as analgesics)

RN 177757-25-4 HCAPLUS

CN Benzeneacetic acid, 4-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]amino]-α-ethyl- (9CI) (CA INDEX NAME)



A

IT 177759-75-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of aromatic amino ethers as analgesics)

RN 177759-75-0 HCAPLUS

CN Benzeneacetic acid, 4-[[[5-bromo-2-(phenylmethoxy)phenyl]methyl]amino]-α-ethyl-, ethyl ester (9CI) (CA INDEX NAME)

Updated Search

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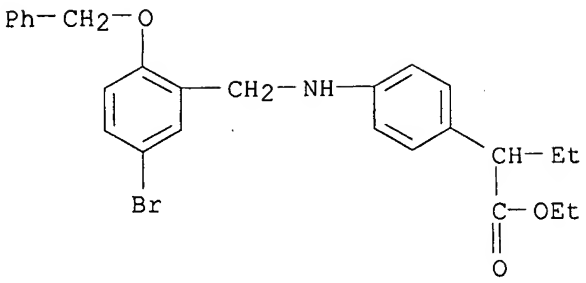

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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
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  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

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  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

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     (FILE 'HOME' ENTERED AT 16:53:07 ON 06 APR 2007)

     FILE 'REGISTRY' ENTERED AT 16:53:12 ON 06 APR 2007
L1              STRUCTURE UPLOADED
L2            0 S L1
L3           13 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 16:56:19 ON 06 APR 2007
L4            3 S L3

     FILE 'CAOLD' ENTERED AT 16:56:31 ON 06 APR 2007
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Updated Search

10572578

=> s l3
L5 0 L3

Updated Search